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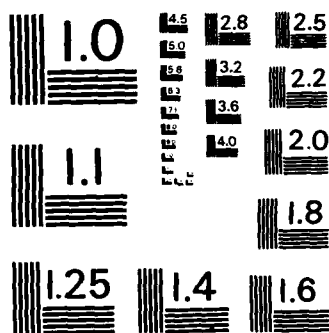
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In  
Atomic  
Spectroscopy

*Report on a Workshop Held in Tucson, Arizona, October 24-26, 1982*

Committee on Line Spectra of the Elements —  
Atomic Spectroscopy  
Commission on Physical Sciences, Mathematics, and Resources  
National Research Council

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Committee on Line Spectra of the Elements-Atomic Spectroscopy  
Commission on Physical Sciences, Mathematics, and Resources  
210 Constitution Avenue, N.W.  
Washington, D.C. 20478

## WORKSHOP PARTICIPANTS

**James J. Wynne**, IBM Thomas J. Watson Research Center,  
*Workshop Chairman*

**Thomas Baer**, Spectra-Physics

**H. Gordon Berry**, Argonne National Laboratory

**James W. Brault**, Kitt Peak National Observatory

**Charles M. Brown**, Naval Research Laboratory, *Topical Panel  
Chairman*

**John G. Conway**, Lawrence Berkeley Laboratory

**Robert D. Cowan**, Los Alamos Scientific Laboratory

**Charles R. Cowley**, University of Michigan

**John L. Hall**, Joint Institute of Laboratory Astrophysics

**Will Happer**, Princeton University

**Serge Haroche**, Ecole Normale Supérieure, Paris, France

**David R. Herrick**, University of Oregon

**Richard A. Keller**, Los Alamos Scientific Laboratory, *Topical  
Panel Chairman*

**Daniel J. Larson**, University of Virginia

**Michael G. Littman**, Princeton University

**Kwang-Tzu Lu**, Argonne National Laboratory

**Joseph H. Macek**, University of Nebraska, *Topical Panel  
Chairman*

**Georgia A. Martin**, National Bureau of Standards, Washington

**William C. Martin**, National Bureau of Standards, Washington

**Thomas J. McIlrath**, University of Maryland, *Topical Panel  
Chairman*

**Robert T. Poe**, University of California, Riverside

**A. Ravi P. Rau**, Louisiana State University, *Topical Panel  
Chairman*

**John Raymond**, Harvard-Smithsonian Center for Astrophysics

**Joseph B. Reader**, National Bureau of Standards, Washington

**William T. Silfvast**, Bell Telephone Laboratories, Holmdel

**Anthony F. Starace**, University of Nebraska

**Stig Stenholm**, University of Helsinki, Finland

**William H. Wing**, University of Arizona

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*James J. Wynne*

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# I. OVERVIEW

## A. Introduction

The study of free oscillations of the electrons in an atom *via* their interaction with electromagnetic radiation, known as atomic spectroscopy, is a modern, active, and *basic* science with core intellectual goals of its own. It also has relevance to a wide cross-section of activities in the physical sciences and to other areas of importance to society. Today, atomic spectroscopy uses modern experimental tools, such as lasers, synchrotron light sources, electron spectrometers, ion traps, and fast ion beams, and advanced approaches to such methods as quantum-defect theory, many-body perturbation theory, and group theory to study the structure of isolated atoms in greater detail and with greater precision than ever before. The effects of collisions, electric and magnetic fields, photoionization, and other interactions between atoms and their environment are now being studied in ways that would have been impossible or forbiddingly complex just a few years ago. An important result of this new work is that atomic spectroscopy has increased its impact on diverse areas of physics as well as the traditional area of the study of the electronic structure of atoms. For example, extensive work on the spectra of highly ionized atoms is vitally important for, as well as motivated by, the desire to investigate and understand vacuum ultraviolet (VUV) spectral observations of high-temperature plasmas from both astrophysical and laboratory sources.

### B. History

Atomic spectroscopy is a field with a long and successful history. At the end of the 19th century, Balmer and Rydberg discovered key regularities and systematics in atomic spectra, which led to Bohr's quantum theory of the hydrogen atom. In the 1920's, atomic spectroscopy had a golden age in connection with the emergence of quantum mechanics and the development of a quantum-mechanical model of atomic structure, capable of explaining major experimentally observable details of atomic spectra. By 1935, a basic foundation had been established, and many physicists turned their attention to the newly emerging problems of nuclear physics and electronics. A monograph by Condon and Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, England, 1935) summarized the field at the time, doing that job so well that it is still a standard reference.

During the next several decades, atomic spectroscopy seemed to be in partial eclipse. In fact, the complex spectra of open-shell atoms were analyzed by a small group of workers, and new theoretical procedures were developed for their interpretation. Two publications, Moore's compilations, *Atomic Energy Levels* (NBS Circular 467, 1949-1958, Vol. I-III), and a review article by Edlen, "Atomic Spectra" (*Handbuch der Physik*, Springer-Verlag, Berlin, 1964, Vol. XXVII, *Spectroscopy I*, pp. 80-220), are notable in giving coherence to the work of this era. Such documents serve the "consumers" of atomic data, e.g., astrophysicists, plasma physicists, and atomic theorists, and have stimulated spectroscopists to examine the problems and shortcomings that these systematic approaches reveal in existing spectral analyses.

The renaissance of atomic spectroscopy began in the 1950's with the impetus of urgent new needs for spectral data in industry, the atomic energy program, the space program, and the Defense Department. The renaissance really gained momentum around 1960, triggered by the development of new light sources,

new detection methods, and rocket and satellite observations and, more subtly, by new theoretical methods.

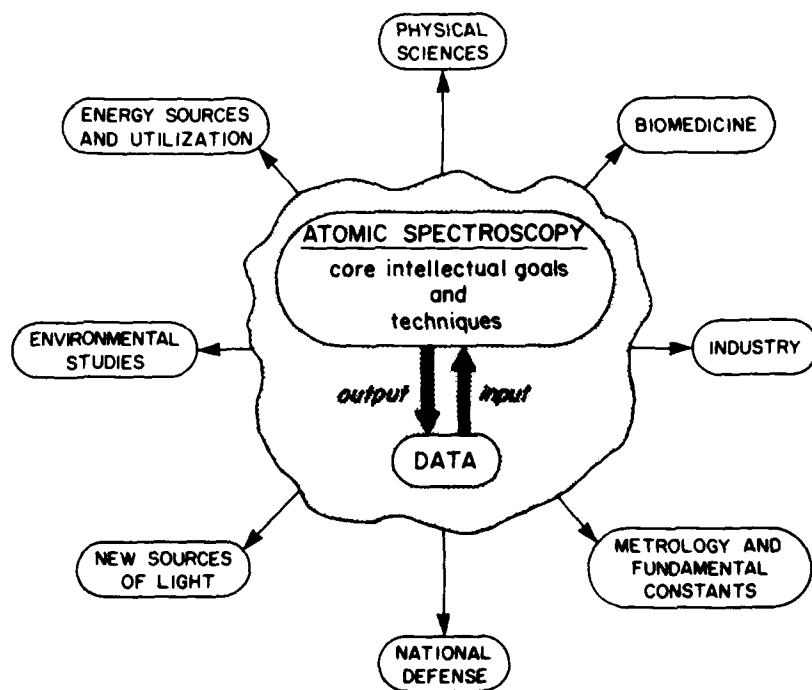
### C. Mission

It is appropriate to step back from the details of the avalanche of new results, adopt a broader perspective, and reflect upon the current status as well as the future of atomic spectroscopy. A workshop was held in Tucson, AZ, from October 24-26, 1982, to produce this report, articulating the collective opinion of the participants on the "state of the art" in current research and on the goals for future research. The workshop was organized under the auspices of the Committee on Line Spectra of the Elements-Atomic Spectroscopy (CLSE-AS) of the National Academy of Sciences-National Research Council (NAS-NRC). The workshop and this report were funded primarily by the National Science Foundation and the Air Force Office of Scientific Research, with additional funds provided by Spectra-Physics and International Business Machines.

### D. Definition and Scope

What is atomic spectroscopy? We define it as the study of atoms (and atomic ions) through their interaction with electromagnetic radiation, in particular, where the radiation is absorbed or emitted with an internal rearrangement of the electrons of the atom. The dependence of these processes on the frequency (or, equivalently, wavelength) of the radiation is called spectroscopy. Excitation or emission of electromagnetic radiation allows atoms to be studied in isolation or in interaction with their environment, including collisional effects. However, collisions are relevant to this report only insofar as they affect the spectra; collisional studies without electromagnetic radiation as a probe are outside of our scope. Molecules, condensed matter, collective effects, surfaces, nuclei, etc., are all within our scope when they are addressed *via* atomic spectroscopy. With this definition, we can look at current research and see if it is

atomic spectroscopy. We quickly find that there are areas of research that clearly fit this category, others that clearly do not fit, and still others that are ambiguous. Thus we come to the notion of a central core of atomic spectroscopy around which we can draw a diffuse border outside of which lie other areas of physical science. We will endeavor to show what constitutes this central core. At the diffuse border we will find extensions of atomic spectroscopy into other areas, such as the spectroscopy of exotic atoms. Outside of the border will be a broad spectrum of activities in the physical sciences.



**FIG. 1** *Atomic spectroscopy, a discipline possessing its own core intellectual issues, has applications to many other areas of science and society.*

## E. Organization and Contents

This report is organized to reflect the above definition and goals (Fig. 1).

At the heart of atomic spectroscopy are the systematics, which are particularly important to the organization and interpretation of the data that are produced. As with any field of science, knowledge should be organized into a systematic scheme. Such a scheme is extremely useful for teaching the field to novices as well as for guiding experts to areas that require further understanding. The beauty of atomic spectroscopy is that quantum mechanics not only established the systematics of the structure due to a single electron moving in a Coulomb potential but provided a framework for systematic investigation of the many-electron atom. It is this many-electron atom and its exquisite mysteries that continue to draw scientists to atomic spectroscopy. Attempts to understand the many-electron atom begin with the spectral regularities previously discovered and move toward trying to find additional regular behavior underlying seemingly irregular (or anomalous) spectra. As this report will show, although there are many unsolved problems, great progress is being made toward uncovering these regularities in the many-electron spectra.

The methods of atomic spectroscopy may be classified under the broad categories of theoretical and experimental techniques. Not only have both categories participated in the renaissance of atomic spectroscopy, but the interplay of theory and experiment has become a necessity in much of the work currently being done. The modern theoretician uses advanced approaches to traditional methods, as well as techniques such as many-electron wave function basis sets, the relativistic random-phase approximation, and R-matrix methods. These approaches allow the theoretician to explain the characteristics of atomic spectra in terms of the underlying structure, gaining deeper and broader insight into the many-electron atom, the prototype of the many-body problem. The modern experimental spectroscopist uses new light sources and atom sources, high-resolution

spectrometers, higher sensitivity detection over wider spectral ranges, and automated data taking and analysis. These research tools allow the experimentalist to accumulate and digest incredible amounts of precise data.

Research in atomic spectroscopy produces primary data, such as atomic line positions (frequencies or wavelengths), widths, strengths (oscillator strengths or atomic transition probabilities), etc., and structural information derived from these data, such as atomic energy levels, ionization limits, etc. Each study produces its own data, which vary as to mode of presentation and accuracy. The data become far more useful when organized into data banks containing refined, evaluated information. Such data compilations are an indispensable addition to the primary research literature and are a critical resource to the experimentalists and theoreticians, providing a base of knowledge upon which new understanding may be built. Thus they provide input back into the central arena of atomic spectroscopy.

The data, together with systematics and theoretical and experimental techniques, constitute the central core of atomic spectroscopy. It is a core that continues to be characterized by the refinement of standard techniques but, of equal importance, features the development of new approaches prompted by expansion in different directions and the relevance to other fields.

The techniques of atomic spectroscopy have long been recognized as useful to other areas of scientific and technological investigation. In many instances, atomic spectroscopy has been the proving ground where these techniques were tested and refined before being applied to other fields. Similarly, atomic spectroscopic data have provided the information base for investigations in other fields. Taking astrophysics as an example, virtually all the experimental data we have on the universe outside of our own solar system have been obtained from atomic (and molecular) spectroscopic observations. Atomic spectroscopy has important applications to problems outside of traditional atomic physics, and progress in many areas is closely tied to improvements in the techniques of atomic spectroscopy and to the availability of more and better data. As shown in Fig. 1,

atomic spectroscopy has applications to many areas of importance to society, and these applications in turn contribute much to the vitality of the field.

The rest of this report has the following content. First, systematics are examined, with an emphasis on core intellectual goals and the search for new conceptual frameworks in which to treat the structure and dynamics of many-electron atoms. Next, theoretical and experimental techniques are examined, stressing the major advances of the past two decades and pointing to new and exciting areas for future investigation. This is followed by a discussion of data, including the status of and needs for critical evaluations and compilations. (Appendices listing existing and planned critical compilations, data centers, published bibliographies, and newsletters are included in this report.) Finally, several areas of application of atomic spectroscopy are highlighted, and many areas of science and technology are assessed from the point of view of their needs for spectroscopic data.

#### **F. Summary and Purpose**

This report expresses the collective opinion of the workshop participants that the areas covered are representative of the best work going on in atomic spectroscopy. In discussing current trends and future goals for research, we have tried to share with the reader our appraisal of where the field is and where it is going. This report has been prepared with the intention that it be an aid to funding agencies in assessing research proposals and to management at research institutions in guiding research carried out in their facilities.

In choosing research areas to highlight, the workshop participants were guided by their own knowledge and experience, and a consensus was often reached as to what areas were most exciting and likely to produce useful results. An unavoidable side effect of imposing strict limits on the length of this report is that some worthwhile areas had to be treated very briefly or even omitted entirely.

## II. SYSTEMATICS OF ATOMIC SPECTRA

### A. Introduction

The search for systematic behavior in existing data and the use of previously discovered systematics in the interpretation of new data are at the heart of atomic spectroscopy. Systematics has repeatedly yielded key new insights into the nature of physical laws. Rydberg's formula for atomic spectral series synthesized large amounts of diverse data and started the physics community on the road to quantum theory. Further studies of systematics led to discoveries of the Pauli exclusion principle and electron spin, just to name two well-known examples. Additionally, the independent-particle model of atoms, indeed of all macroscopic matter, and atomic systematics are closely intertwined. Group theory, which forms such an essential part of modern physical theories, was brought into physics to systematize the symmetry properties of atomic states.

We now largely understand the fundamental dynamical laws, namely, quantum electrodynamics (QED) and all of its approximate versions, that, in principle, govern atomic structure and dynamics. Modern study of atomic systematics has repeatedly demonstrated, however, that the standard independent-particle model must be augmented by new concepts, reformulated in terms appropriate to new spectral regions, or, in many

instances, abandoned altogether. The search for new conceptual frameworks within which to fit data of ever-increasing precision in ever-wider spectral regions forms the key intellectual challenge of atomic spectroscopy, generally, and atomic systematics, in particular. This search is greatly aided by the probing of regularities and, perhaps even more importantly, the conspicuous irregularities of atomic spectral distributions.

Modern studies of such distributions differ qualitatively from those that provided the initial synthesis of the quantum theory. With the help of novel experimental techniques, it is now possible to select atomic species and atomic states so as to control the relative strengths of different interactions and thus focus on features that need to be incorporated into the conceptual framework. For a given species, the degree of excitation (principal quantum number) and, often, other degrees of freedom, such as the angular momentum, are selectable over a wide range. The charge of the nucleus, the number of its neutrons, and the valence shell structure of the atom can also be selected and varied over a wide range of ionic or atomic species so as to exhibit the evolution of spectral properties as these features are progressively modified. The very nature of the particles building the atomic system can also be changed by preparing "exotic" systems made of leptons or hadrons other than electrons, protons, and neutrons (e.g., positronium, muonium, muonic atoms...).

The selectivity thus achieved also makes possible the systematic use of atoms as probes for a variety of interactions not primarily concerned with atomic dynamics: the study of stable or unstable nuclear structure (*via* hyperfine-structure measurements); the test of parity-violating terms in electron-nucleus interactions in the context of the unification of the weak and electromagnetic interactions; and the interactions with other atoms, molecules, and surfaces. The scope of these activities appears *limitless*. If recent history is a guide, we can expect that future technical developments will continue to broaden the horizons of atomic spectroscopy and provide new challenges to our conceptual frameworks.

**B. Examples of Systematics**

Atomic systematics divide naturally into two parts, namely, those aspects that relate to isolated atoms and those aspects that relate to changing environments and external perturbations. Both aspects are illustrated by some current trends in atomic spectroscopy. The following examples are selected to illustrate systematic studies in various spectral ranges, beginning with the optical and infrared region, proceeding to the vacuum ultraviolet (VUV), and concluding with the x-ray region.

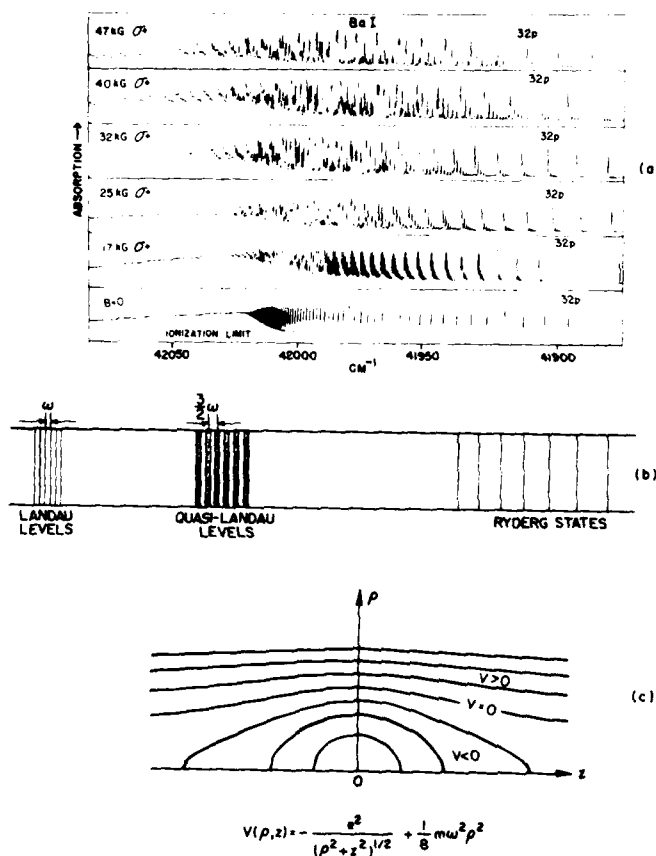
**1. Weakly Bound Species**

The electron-atomic core interaction and the effects of external fields and collisions may be studied with unprecedented levels of precision by preparing and manipulating a wide variety of weakly bound species, including atoms in high Rydberg levels and negative ions. Wavefunctions of Rydberg electrons bound to an ion core are shifted in phase relative to those appropriate to hydrogen-like species. These phase shifts, which reflect the perturbing effect of the short-range interaction with the core electrons, can be expressed in terms of the "quantum defect" which appears in the Rydberg formula for the energy levels of the bound states. Quantum-defect analysis points out the continuity between bound and continuum states, the latter lying above the ionization limit in a domain where scattering amplitudes have traditionally been described in terms of phase shifts. In this respect, Rydberg atoms can be considered as systems in which a low-energy electron is scattered off the ion core, allowing us to extract very valuable information about the properties of the core. For example, dipolar and quadrupolar polarizabilities of the core are inferred from Rydberg spectroscopy measurements. Rydberg-level phase shifts or, equivalently, quantum defects have been determined to six or seven significant figures, a remarkable level of precision for measurements of this kind, and possible only in atomic spectroscopy.

A newer aspect of the weakly-bound Rydberg system is the possibility of varying almost continuously the atomic size by exciting the valence electron closer and closer to the ionization limit. With laser and atomic beam techniques, excited states whose orbitals are as large as a fraction of a micron (a biological size!) and whose binding energies are sub-thermal are currently being studied. Spectroscopic properties related to the atomic size and binding energy are quantitatively very different for quantum states in this region than for much lower-lying states. For example, the interaction between relatively small electric or magnetic fields and the Rydberg electron can become of the same order of magnitude or even larger than the  $1/r$  Coulombic interaction between the ion core and the Rydberg electron, leading to an extremely strong modification of the Rydberg spectrum. (This is an example of a topic that lies in the diffuse border separating atomic spectroscopy from other areas of physical science.)

The case of an external magnetic field is of particular current interest. The evolution from the Rydberg spectrum to a Landau-like spectrum (characterized by resonances of approximately equal spacing, that spacing being proportional to the magnetic field) has been studied as one continuously increases the electron energy past the ionization level (Fig. 2). The theory of this effect is still incomplete, and the basic problem of a hydrogen atom in the presence of a magnetic field of arbitrary amplitude is still not solved in its full generality. (See Chapter III, Section C4 for further discussion.) This effect has astrophysical significance, since one expects excited atoms in the vicinity of neutron stars to experience extremely strong magnetic fields. Thus Rydberg atoms allow us to investigate the effects of extreme environments on the systematic behavior of atoms.

Closely related to these studies, the measurement of photodetachment spectra of negative ions in a magnetic field also illustrates the rich structure in the oscillator strength distribution of loosely bound systems in external fields. Here, again, a Landau-like structure is observed, but at much lower fields



**FIG. 2** Electronic motion in combined Coulomb and magnetic fields:

(a) Absorption spectra of barium (Ba I) showing  $1P_1^0$  Rydberg series for different magnetic fields (B). The spectra are taken in  $\sigma_+$  ( $m=1$ ) polarization. At any B field, the states toward the right of the diagram show a quadratic Zeeman shift to higher energies. Progressing towards the left, the breakdown first of  $l$  and then of  $n$  as good quantum numbers leads to a splitting of the zero-field levels. Note the equally spaced resonances (quasi-Landau levels) around the ionization limit;

(b) Schematic rendering of spectrum for  $B=25$  kG, emphasizing three characteristic regimes: (1) the Rydberg levels at lower energies, where the Coulomb field dominates; (2) the equally spaced (quasi-Landau) resonances, with spacing equal to  $3\omega/2$  (where  $\omega = eB/mc$  is the cyclotron frequency), around the ionization limit, where neither field dominates; and (3) the Landau levels, with spacing  $\omega$  (not exhibited clearly in (a)), at much higher energies, where the magnetic field dominates;

(c) Combined Coulomb and diamagnetic potential with a sketch of equipotentials in the two-dimensional space  $p, z$  ( $B$  is parallel to  $z$ ). The motion of an electron in such a non-separable potential leads to the observed spectrum.

than in the Rydberg atom case. The interaction of the continuum electron with the neutral atomic core of the negative ion is indeed much weaker than the Coulombic interaction with the ionic core of the Rydberg atom, resulting in a stronger effect of the magnetic field.

The case of an external electric (Stark) field is also of interest. The interplay of the Coulomb and Stark fields also produces resonances in the normally smooth continuum. This effect has practical significance since Stark field ionization has been widely adapted as a detection method in laser spectroscopy of atoms.

The radiative behavior of Rydberg atoms also changes continuously with the atomic size and binding energy. The density of bound states increases as one gets closer to ionization, thereby enabling the atoms to resonantly interact with radiation of increasing wavelengths (far-infrared and millimeter waves). Also, the electric dipole matrix elements of the corresponding transitions become extremely large. Systematic studies of these radiative properties are being investigated, in view of possible application to infrared radiation detector technology (see Chapter IV, Section B3).

Finally, the effect of collision processes on Rydberg atom spectra is another area in which systematic studies are being performed. Here, again, the possibility of selecting atomic states and transition frequencies opens the door to the study of well-controlled processes. For example, resonant features are observed when two Rydberg atoms interact with a microwave field at a frequency matching a frequency *difference* between two different transitions, one in each atom, revealing resonant energy transfer between colliding atoms in the presence of the radiation field.

## 2. Sequences

Comparisons of spectra along several types of sequences prove fruitful for systematic studies: (a) isoelectronic sequences, i.e., successive ionic species with the same number of

electrons (e.g.,  $H^-$ , He,  $Li^+$ , etc.), (b) isonuclear sequences, i.e., species having identical nuclei but differing numbers of external electrons (e.g., Li,  $Li^+$ ,  $Li^{++}$ ), and (c) homologous sequences, i.e., atomic species having the same number of valence electrons (e.g., Li, Na, K, etc.). Studies concentrate on the regularly varying spectral distributions of oscillator strength expected, and generally found, along atomic sequences. The usual regularity contrasts with notable irregularities and redistributions of atomic spectral distributions, thus pointing to areas for further study.

#### **a. Isoelectronic Sequences**

Isoelectronic comparison of photoabsorption from the ground state of Xe,  $Cs^+$ , and  $Ba^{++}$  reveals that the interaction of the excited electron with the atomic core changes dramatically along the sequence (Fig. 3). This is reflected in a rapid redistribution of oscillator strength, as illustrated by the narrowing of an autoionizing resonance as one moves from Xe to  $Ba^{++}$ . The theoretical interpretation of this behavior has been provided by an approach that emphasizes radical changes in electron correlations and autoionizing lifetimes, along the sequence. This study depended on the ability to prepare specific ionic species by laser-driven ionization and on the development of theoretical methods that were capable of treating the observed spectra. Such methods, in this case multichannel quantum defect theory (MQDT) coupled with the relativistic random-phase approximation (RRPA), illustrate the increasing sophistication with which theoreticians can treat many-electron effects in atoms.

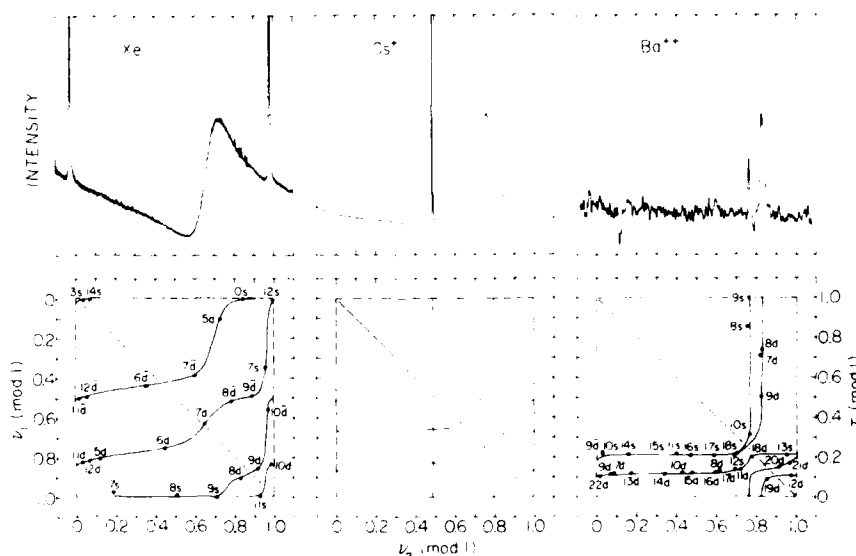
#### **b. Isonuclear Sequences**

Photoabsorption resulting in the excitation of a 4d electron in the Ba,  $Ba^+$ ,  $Ba^{++}$  isonuclear sequence illustrates the expected similarity between Ba and  $Ba^+$  and a striking difference in  $Ba^{++}$  (Fig. 4). Again, this observation is made possible by laser ionization of Ba to produce selected ionic species. The observed redistribution may be understood in terms of the sud-

den contraction of the (unoccupied) 4f orbitals as the outer electrons of Ba are removed. This contraction of 4f orbitals is a ubiquitous feature of the spectra of atoms near the beginning of the sixth row of the periodic table and, in this instance, results from moving along the Ba isonuclear sequence, thereby changing the effective potential seen by the 4f orbitals.

### c. Homologous Sequences

The properties of complex Rydberg and autoionization spectra of noble gas atoms (Ne, Ar, Kr, and Xe), such as energy



**FIG. 3** Upper figures: Photoabsorption spectra, in the autoionization continuum, of the isoelectronic sequence Xe, Cs<sup>+</sup>, and Ba<sup>++</sup>. Lower figures: Corresponding Lu-Fano (MQDT) plots of effective quantum numbers,  $\nu_1$  vs.  $\nu_2$ , where  $\nu_1$  is determined using the lowest (<sup>2</sup>P<sub>3/2</sub>) ionization limit and  $\nu_2$  is determined using the next higher (<sup>2</sup>P<sub>1/2</sub>) ionization limit. These plots represent one cycle in  $\nu_2$  (i.e.,  $\nu_2$  changes by an integer) and show comparable structure for all three species. The systematics depicted is the redistribution of oscillator strength, illustrated by the narrowing of the d-like autoionizing resonances (the broader peaks) as one moves from Xe to Ba<sup>++</sup>. (The narrower peaks in the spectra are s-like autoionizing resonances.)

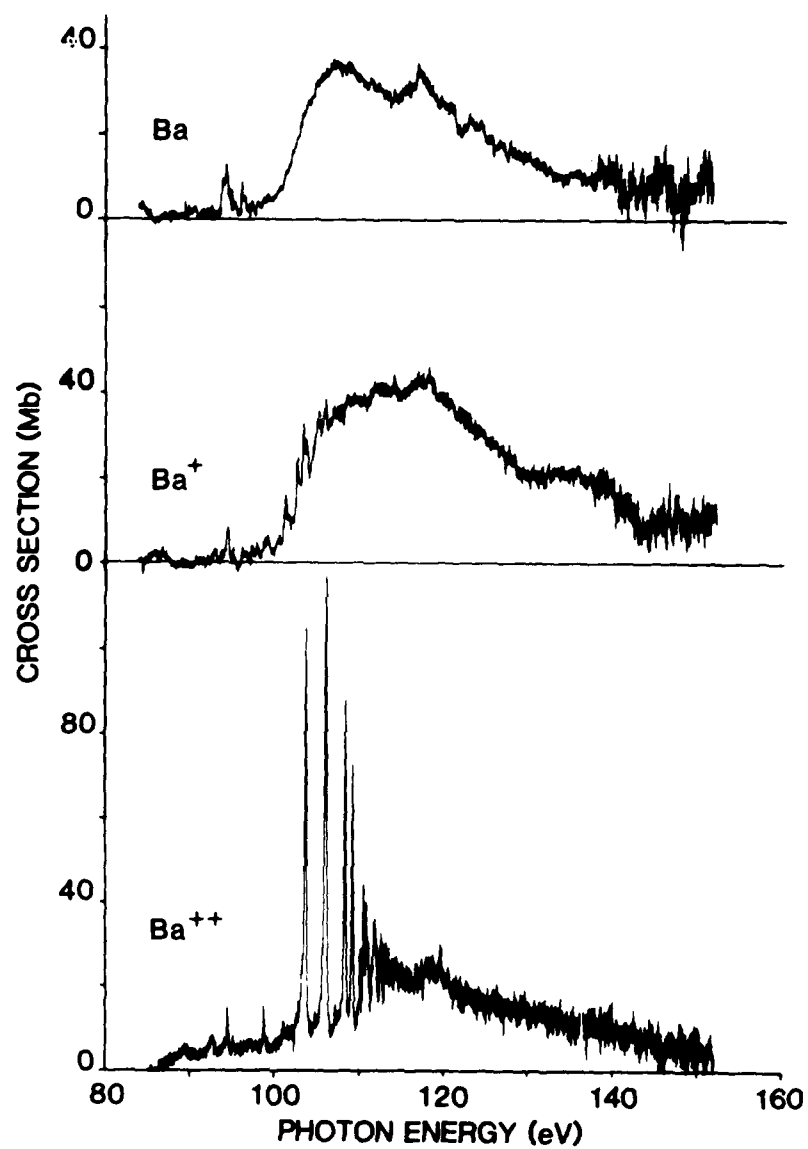


FIG. 4 Photoabsorption cross sections for  $4d \rightarrow nf, ef$  transitions in the isonuclear sequence,  $Ba$ ,  $Ba^+$ , and  $Ba^{++}$ . The systematics depicted is the similarity between  $Ba$  and  $Ba^+$ , and the striking difference for  $Ba^{++}$ . The observed redistribution of oscillator strength is interpreted as due to the partial contraction of the  $4f$  orbital as the outer electrons of  $Ba$  are removed.

levels, oscillator strengths, lifetimes, and autoionization linewidths, have been successfully characterized by MQDT, a method that treats the Rydberg spectra and the autoionizing continuum in a unified way. For example, the observed increase of autoionizing linewidths with increasing atomic number was explained to be a consequence of the increase in the spin-orbit interaction leading to stronger channel interaction in the framework of MQDT. The extension of such studies to the Be group reveals an interesting and general effect, namely, the hybridization of singly excited states and doubly excited states, due to electron correlation, not only for low-lying excited states but also in the high excitation and continuum regions. One consequence of hybridization between these two contrasting orbitals is an anomalous intensity distribution. For Be and Mg, the hybridization between the Rydberg channel  $nsn'p$  and the doubly excited channel  $nnp'n's$  extends from the discrete region into the continuum. For Ca, Sr, and Ba, the dominant interaction is between the  $sp$  and  $dp$  channels and is characterized by a common set of quantum defect parameters.

We know that the alkaline earth atoms in their ground states are more active chemically than the noble gases. This is related to the fact that their electronic ground states are not pure closed-shell configurations ( $s^2$ ) but contain admixtures of open-shell configurations ( $p^2$  and  $d^2$ ). The perspective gained from spectroscopic studies of excited states may lead to a better understanding of the chemical reactions of electronically excited atomic species. The C-group and F-group elements provide unique and exciting opportunities for such studies.

The complications in the many-body dynamical theory for open-shell atoms and the necessity of including several configurations in the ground state wavefunctions make these atoms especially intractable. Furthermore, many of the open-shell atoms do not have ground states with total angular momentum  $J=0$ . This fact greatly increases the difficulty in determining the  $J$  of final states excited from the ground state, in particular for continuum spectra. Thus, extensive work remains to be done on

the open-shell atoms before their regularities along homologous sequences can be recognized.

### 3. Multielectron Excitation

Multiple excitation of atoms and ions prepares states in which two (or more) electrons share excitation energy almost equally. Such states are particularly sensitive to electron-electron correlation. The two- or three-electron species  $H^-$ ,  $He$ , and  $He^-$  manifest this correlation with a minimum of competition arising from interactions of excited electrons with the core. Because two electrons move outside of the atomic core, these systems are not well-characterized by an independent-particle framework and must be treated by methods that intrinsically account for the joint motion of both electrons. This subject is in a stage of intense development (see Chapter III, Section C3).

In the case of  $H^-$ , where photoabsorption measurements have revealed the doubly excited, autoionizing states, particular emphasis on the threshold for simultaneous ejection of two electrons has substantiated the dominant effect of electron correlation. Since this spectral region is becoming accessible by VUV laser-based techniques, one can anticipate further improvements in precision and selectivity. Similar remarks apply to the photoionization of  $He^-$ , where such measurements complement those in  $H^-$ . For example, when two electrons are ejected from  $He^-$ , their spins are aligned parallel, and thus the triplet mode of motion of the two outgoing electrons is probed; in contrast, for  $H^-$ , only the singlet mode is probed.

### 4. X-ray Transitions

The dependence on atomic number of the energies of particular x-ray transitions is a classic example of extremely regular behavior. Recent determinations of  $K\alpha$  and  $K\beta$  wavelengths at accuracy levels of a few parts in  $10^6$  or better generally agree with theoretical predictions but also reveal 1-2eV discrepancies in the medium to heavy element range. This de-

parture is expected due to the effects of electron correlations not accounted for in the existing theory.

Studies of x-ray line strengths reveal striking irregularities at specific places in the periodic table. In some instances, an x-ray line unexpectedly disappears altogether. This abrupt discontinuity of atomic spectral properties is traced to the onset of energetically allowed rearrangements of atomic electrons leading to removal of excitation energy by non-radiative transitions. Here electron correlations play a central role in producing the remarkable redistribution of oscillator strength.

### III. THEORETICAL TECHNIQUES

#### A. Introduction

The continued refinement of standard theoretical techniques to give more accurate values for quantities of spectroscopic interest is a vital part of atomic spectroscopy. Equally important is the development of new techniques prompted by expansion of the field in different directions. Historically, atomic spectroscopy had a direct role in the development of Racah algebra and, more broadly, of the basic elements of quantum mechanics. The study of spectra in external fields led to the development of perturbation theory. In generating these techniques, a process that continues today, atomic spectroscopy provides methods of interest to the broader area of theoretical physics in general. The established techniques for working out atomic structure apply to other spectroscopies as well, whether it be for excitons, impurity states, and two-dimensional systems in condensed-matter physics, or charmonium and other quarkonium states in particle physics. All these bound states are described in the same language, and their eigenvalues and wavefunctions calculated in the same way as in atoms. Even more significantly, the study of highly correlated structures, such as multiply excited states in atoms or highly excited Rydberg states in external fields, is leading to the development of theoretical techniques that will be applicable generally in physics. The study of atomic systems, where the basic interactions are well-understood, yields insights into general properties of non-

separable dynamical systems which are of much current interest elsewhere in the study of nonlinear physics.

Even though the basic interactions are known, the long range of the Coulomb interaction leads to difficulties in theoretical calculations. First, a very large number of states is involved, particularly with increasing excitation, and correlations and interaction extend over large distances. Second, in a heavy atom, the outer electrons are often poorly described. This is particularly so when one asks for detailed questions about the wavefunction, such as its behavior near the origin, which may contribute little to the energy but which is crucial for applications in nuclear (hyperfine structure) and particle physics (weak-interaction parity-violation effects). Thus, having said that the Hamiltonian is known and the atom is, in principle, calculable, theory still remains challenging, necessitating new and specific developments for each application.

#### **B. Areas of Current Interest**

As in any other field of theoretical physics, new theoretical techniques in atomic spectroscopy arise to address questions generated by experimental developments that probe, in increasingly sophisticated ways, the structure and dynamics of atoms:

1. The study of increasingly higher excitation means more channels are accessed, particularly those involving multiple-electron excitation. The correlation between electrons has then to be treated to increasing levels of significance. The general development of theory (Section C) features the departure from the basic independent-particle picture of atomic electrons to multi-configuration interactions and then to a description that focuses, even at the starting level, on a pair (or more) of electrons as the fundamental entity.
2. Primarily because of developments in the fusion program and in heavy-ion acceleration capability, the treatment of highly stripped species and, therefore, stronger relativistic effects for the outer electrons (stemming from the stronger Coulomb fields) has had to be increasingly emphasized (Section C1).

3. Increasingly complete experimental information (angular distribution, spin polarization) on continuum states, which are closely related to high-lying, bound, Rydberg states (Section C2), requires a more detailed theoretical description of the wavefunctions.
4. Increasing brightness of laser light sources has given rise to the study of nonlinear responses of an atomic system and the inclusion of the electromagnetic field on an equal footing as a dynamical variable in the problem (Section C4b).
5. The technology of handling new and exotic species, such as muonic helium ( $\alpha + {}^2\mu^- e^-$ ) and geonium (an electron held in a trap of electric and magnetic fields), has motivated the extension of theoretical spectroscopic calculations to higher precision (Section D1).

### C. Techniques

#### 1. Self-Consistent-Field Methods

For energies and wavefunctions of low-lying levels, the central-field model of the atom leads to the use of basis functions consisting of linear combinations of products of one-electron spin-orbitals, obtained by self-consistent-field (SCF) solutions of the Hartree-Fock equations. The strong interaction between electrons, mainly at small distances, means that a single configuration is inadequate. Therefore, electron-correlation effects are explicitly taken into account *via* configuration-interaction (CI) methods.

The SCF approach provides a straightforward general method of computing large numbers of energy levels, wavelengths, and transition probabilities within modest basis sets of functions. For moderately complex structures, the accuracy of computed excitation and ionization energies for neutral and weakly ionized atoms is typically 2 to 5%. For ten- or more-fold ionized atoms, the accuracy is  $\sim 0.1$  to 0.3% for ionization and for transitions with  $\Delta n \neq 0$  and 1 to 2% for transitions with  $\Delta n = 0$ . Quantities other than energy levels, computed from the

atomic wavefunctions, are less accurate, perhaps 10 to 30% for oscillator strengths of strong lines and order-of-magnitude inaccuracies for weak lines suffering serious destructive-interference cancellation between competing amplitudes.

Relativistic effects are already non-negligible for  $Z \sim 10$  and are evaluated by perturbation theory. But their growing importance with increasing  $Z$  means that for values of  $Z$  greater than  $\sim 60$ , it is best to go to fully relativistic, Dirac-Fock SCF calculations, with the addition of Breit (magnetic-plus-retardation) and Lamb-shift (electron-self-energy and vacuum polarization) energy corrections. These extremely laborious self-energy calculations have as yet been carried out only for 1s, 2s, and 2p states of one-electron ions and for 1s electrons of many-electron atoms.

## 2. Collision Theory Description - MQDT

In the region near the lowest ionization thresholds, correlation effects *dominate* the observed spectra. Because of the high excitation and the large density of states involved, a large number of configurations need to be included in the SCF-CI approach. This number diverges, making the extension to the vicinity of the ionization threshold impossible. Instead, one adopts an alternative approach, treating not individual energy states but a whole channel of them (with energy a running index), much as in scattering or collision theory.

In fact, given the much stronger Coulomb potential at small  $r$ , electron-ion scattering amplitudes vary only slowly with the excited electron's kinetic energy, which is much smaller in comparison. As a result, given the scattering amplitudes, the extremely rich spectra (an infinite number of energy levels) below and above ionization thresholds can be described theoretically in great detail using analytic properties of Coulomb wavefunctions and a small number of parameters characterizing the non-Coulomb interactions at small  $r$ . Such a treatment in the framework of electron-ion collision theory is the basis of multi-channel quantum defect theory (MQDT) which may also be

used semiempirically to classify and analyze experimental spectral data.

The parameters characterizing the short-range interactions can be obtained by fitting to the experimental data. Alternatively, the required MQDT parameters can be determined by any of a variety of *ab initio* theoretical methods. Thus, many methods in scattering theory - close-coupling, random-phase approximation, or many-body perturbation theory - can be used to obtain transition amplitudes just above threshold. Then the MQDT parameters may be extracted and used to predict the system's spectroscopic behavior below threshold. Such *ab initio* calculations for closed-shell atoms can now also include relativistic effects by means of the relativistic random-phase approximation (RRPA). Extension of the theory to open-shell atoms is underway. The MQDT parameters may also be calculated directly by so-called R-matrix type theoretical methods, which diagonalize the exact Hamiltonian within a large basis of discrete, inner-region, basis states.

### 3. Novel Two-Electron Basis States

With even higher excitations, particularly in the vicinity of doubly excited states, correlations become entirely dominant. Extensive CI bases (Section C1) and other approaches (Section D2) have provided fairly accurate results for specific states. But with the increasing numerical complexity involved, it seems impossible to extend these methods to cover many atoms and/or higher-lying, doubly excited, and multiply excited states because of the divergence in the number of states and even in the number of channels. The unusually strong correlation has suggested instead that one abandon the traditional independent-electron model and recast theory in terms of pictures that focus on two electrons at the outset.

### a. Alternative Two-Electron Coordinates

When CI wavefunctions of doubly excited states are plotted in terms of a radius  $R^2 = (r_1^2 + r_2^2)$  and a pseudo-angle  $\alpha = \arctan(r_2/r_1)$  in place of  $r_1$  and  $r_2$ , the radial coordinates of the two excited electrons, one finds that nodal lines lie approximately in regions characterized by constant  $R$  and constant  $\alpha$ . Such a nodal pattern implies that  $R$  and  $\alpha$  are quasi-separable coordinates, a result that is exploited by the so-called "hyperspherical" coordinate method; the set  $(R, \alpha, \hat{r}_1, \hat{r}_2)$  represents the spherical coordinates of the six-dimensional space spanned by  $(r_1, r_2)$ .

The strong electron correlation in doubly excited states seems, therefore, to call for moving away from the independent-electron picture even in the very choice of coordinates:  $R, \alpha$ . The quasi-separability, in terms of an adiabatic separation of the two-electron Schrödinger equation, with the motion in  $\alpha$  much faster than in  $R$ , has successfully accounted for the energies and widths of low-lying doubly excited states. The results agree well with predictions obtained by elaborate close-coupling calculations and with experiment.

In the extension to really high-lying, two-electron levels, close to the double ionization limit of the atom, the adiabatic hyperspherical approach fails, and new features of the correlations come into play. A guideline on how to proceed is provided by the study of threshold laws for double ionization. This study has pointed to a special role for the region of configuration space that corresponds to the two electrons having roughly equal (that is,  $\alpha \cong \pi/4$ ) and oppositely directed radius vectors. The total potential on the surface of a hypersphere displays a ridge in  $\alpha$  in this region. The key concept that has emerged is that the concentration of the wavefunction in this region increases with higher excitation and becomes a quasi-localization as the double ionization limit is approached. This feature and attendant implications for incorporating the effects of a large number of states are physical concepts of perhaps very broad relevance (see also Section C4a).

**b. Alternative Algebraic Basis Sets**

When CI calculations of doubly excited states are examined, one finds two or more basis configurations contributing with comparable strengths. Further, the mixings are just what one obtains on the basis of certain group multiplications. Thus, one approach starts with the well-known exact symmetry under the four-dimensional rotation group  $O(4)$  of degenerate excited orbitals of  $\text{He}^+$  and  $\text{H}$ . Besides the angular momentum  $I$ , the Runge-Lenz vector  $\mathbf{b}$  provides the generators of  $O(4)$ . Since an  $O(4)$  representation includes the alternative  $I$  values at that energy, coupling  $O(4)$  groups for the two electrons leads to correlated wavefunctions with angular correlation as reflected in the mixing of  $I$ . Specifically,  $I_1$  and  $I_2$  are mixed by coupling the difference of Runge-Lenz vectors,  $\mathbf{B}$ , with  $\mathbf{L} = \mathbf{I}_1 + \mathbf{I}_2$ . The coupled states are bases for representations of the  $O(4)$  group with  $\mathbf{B}^2$  and  $\mathbf{L} \cdot \mathbf{B}$  diagonal, and these operators are approximate constants of the motion. When the ordinary CI data are re-analyzed in the  $O(4)$  basis, new systematic blocks of levels called "multiplets" and "supermultiplets" are obtained according to different hierarchies of  $O(4)$  symmetry labels. Contact with the hyperspherical channel structure can also be made by a similar  $O(4)$  classification of the large- $R$  region of the effective potentials.

The symmetry approach has uncovered many regularities that are otherwise "hidden." Most important are progressions of  $L$ -excitations and groupings of levels into supermultiplets that are very similar to rotations and vibrations of a linear triatomic molecule. The  $O(4)$  symmetry ideas have thus forged a new link between coupled states of atoms in molecules, on the one hand, and strongly correlated electronic states in atoms, on the other hand. There are other links with nuclear spectroscopy, where the concepts of collective rotations and vibrations, described by approximate symmetries, and the interacting Boson model, with its focus on pairs of particles, are already familiar.

So far, the greatest value of applying symmetry ideas to the case of doubly excited states of atoms has been the efficient

organization of a wide range of theoretical data. Experimental mapping of the spectra remains far from complete, however, especially in the higher-L regime where direct access from the ground state is limited.

#### **4. Strong Coupling Between Atoms and External Fields**

In the presence of strong external fields, the electronic structure of an atom may be significantly modified. This topic lies in the diffuse region separating atomic spectroscopy from other areas of physical science (see Fig. 1).

##### **a. Static Fields**

For highly excited Rydberg states of atoms that are subjected to laboratory magnetic and/or electric fields, neither the Coulomb nor the external field can be considered perturbative. There is a highly correlated motion of the electron in the non-separable potential obtained by superposing the two fields. The experimental evidence is that such a motion gives rise to broad resonances that dominate the spectrum around the ionization threshold of the atom (see Fig. 2). The theoretical analysis of this problem has much in common with that of high-lying, doubly excited atomic states in the neighborhood of the double ionization threshold, discussed in Section C3a. The same concept of a localization of the wavefunction in the vicinity of a ridge of the potential seems to be involved. Indicative of the wider significance of non-separable problems of atomic spectra in external fields is that modern semi-classical trajectory calculations for the quantization of non-integrable systems have found these problems to be a testing ground for their techniques.

These external field effects, depending as they do on the size of the excited state, are of importance as diagnostic tools for distinguishing between excited states. Electric field ionization is already an example of such state selection. Furthermore, magnetic fields may have a particularly useful role in untangling the effects of multiply excited from singly excited states in

complex spectra, such as that of Ba discussed in Chapter II, Section B1 (Fig. 2).

### **b. Radiation Fields: Laser Spectroscopy**

Spectroscopy with lasers introduces new methods and concepts. Coherent laser spectroscopy differs from coherent radio-frequency spectroscopy because of (1) the much shorter wavelength of the radiation, (2) the importance of spontaneous emission, and (3) the observable effect of photon recoil. The narrow spectral width of the laser allows it to act on a few energy levels selectively, and these may be strongly modified by the high optical fields.

The short wavelength and narrow spectral width of laser light make it necessary to consider velocity and spatial inhomogeneities throughout the atomic medium. One gets so-called "hole burning" effects when one resonantly excites atoms with only a given velocity or spatial position. The experimental observations of saturation and polarization spectroscopy can be analyzed for the influence of power broadening and shifts, ac Stark effects, coherent vs. incoherent contributions, and collisional perturbations.

The high intensities of lasers severely limit the applicability of perturbation approaches. The spectral distribution of spontaneous emission is modified, and optical pumping effects become an essential part of the phenomena. To describe these effects, one must add to the treatment of atomic levels the quantum states of the electromagnetic field and consider the coupled atomic-electromagnetic field system - the so-called "dressed atom" system. Density matrix techniques prove convenient for this treatment. Photon statistics may be important, and quasi-probability techniques are used to treat them.

The exchange of momentum in individual photon absorption and emission events causes observable recoil effects, modifying the velocity and spatial distribution of the atoms. The coupling between internal (i.e., electronic excitation) and external (i.e., translational) degrees of freedom of the atom needs to

be taken into account both for theoretical interpretation and for achieving laser cooling of atoms (see Chapter IV, Section B2).

The high intensities used for multiphoton spectroscopy necessitate going beyond the lowest orders in perturbation theory. Near the ionization threshold, the mixing of several processes can cause field-induced structures in the continuum, with characteristically asymmetric "Fano lineshapes."

#### **D. More Specialized Spectroscopies**

In Section C we have described rather general theoretical approaches for treating the interaction of a single photon with the outer electrons of a given atomic/ionic configuration. Here we describe briefly some more specialized topics.

##### **1. Quantum Electrodynamic Theory**

The atom has long been of interest as a laboratory for testing quantum electrodynamic (QED) corrections to the energy levels. In all but the simplest systems, namely one-electron atoms, theoretical calculations of atomic spectra are not yet accurate enough for this purpose. In hydrogen and high- $Z$ , one-electron (hydrogenic) atoms, the accuracy of Lamb-shift tests has considerably improved over the years. In muonic helium, the ground state hyperfine structure has gone from being unknown to being determined to one part in  $10^4$ . A technique that has been useful in this context, namely, the expansion of the Coulomb Green's function in partial waves for the purpose of calculating radiative corrections, may find application elsewhere as well. For instance, intense radiation field effects, discussed in Section C4b, also involve summing over large numbers of excited states, so that descriptions *via* Green's functions, or techniques for approximating them, are important.

## **2. Techniques Imported from Other Areas**

Atomic spectroscopy has played the role of a proving ground for mathematical techniques developed in other areas of physics. The study of non-integrable motion in classical systems has already been mentioned in Section C4a. Resummation techniques, such as Padé approximants and Borel summation, of interest in field theory, have used the Stark effect in hydrogen as a test case, with impressive agreement between theory and experiment. For Stark resonances and doubly excited states, there have been calculations involving complex coordinates. Very accurate values for the positions and widths of some doubly excited states, based on numerical diagonalization of large basis sets, have been obtained. Another method, also borrowed from field theory, is the use of  $1/N$  expansions where  $N$  is the spatial dimension of the problem. Applications to date have been confined to very simple cases. Lastly, there is the density-functional method, which originated in solid-state physics and has now seen some applications to atoms.

## **IV. EXPERIMENTAL TECHNIQUES**

### **A. Introduction**

Atomic spectroscopy originated in the measurement of the properties of spectral lines. Such basic measurements remain a strong necessity and active part of the field. However, this area has evolved with new experimental techniques made possible by new light sources, precise control of the atomic environment, state-of-the-art electronics, computers, novel methods of source preparation, and other supportive skills. These techniques have allowed scientists to achieve higher precision in the determination of line positions, higher time resolution in the measurement of dynamic properties, and higher sensitivity to small numbers of atoms or photons. Moreover, the application of such new techniques continues to lead to discoveries of qualitatively new physical processes.

### **B. Spectroscopic Techniques**

A representative set of current trends that illustrate the range and power of the new techniques is presented below.

#### **1. Extension of Tunable Laser Techniques to the Vacuum Ultraviolet**

The dye laser has revolutionized spectroscopy in the entire region from the near infrared to the near ultraviolet by

providing a source of tunable, spectrally narrow radiation of unprecedented brightness. The literature of the past decade abounds with novel spectroscopic studies made possible by dye lasers. Frequency-doubling techniques routinely provide coherent light generation up to frequencies of  $\sim 46,000 \text{ cm}^{-1}$ . But the extension of such techniques to higher frequencies is prevented by the lack of acentric crystals suitable for frequency doubling into the VUV. Thus alternate methods are being studied for the generation of intense, tunable light in the VUV.

One technique is based on coherent, nonlinear optical sum mixing of dye lasers in a phase-matched atomic vapor. Coverage from  $\sim 50,000$  to  $\sim 100,000 \text{ cm}^{-1}$  has been achieved. Spectra may be obtained by using this light as a bright source for absorption or photoionization studies. Alternatively, the VUV generation process shows enhancement as one tunes through the resonances of the atomic vapor that forms the nonlinear medium. The enhancement, including its lineshape, provides information about the electronic structure of the atoms that complements that obtained by absorption or photoionization techniques.

In another technique, metastable He atoms are irradiated by a pulsed, spectrally narrow, tunable dye laser, and, *via* an anti-Stokes Raman process, radiation is generated at the sum of the energies of the excited He atoms ( $166277 \text{ cm}^{-1}$ ) and the dye laser photons, with a spectral width limited by the Doppler width of the He atoms. The anti-Stokes source has been used to obtain an absorption spectrum of potassium vapor from  $\sim 179000$  to  $\sim 187000 \text{ cm}^{-1}$ , and inner-shell absorption features were observed with high resolution. Despite the fact that this region had previously been studied with spectrographs, several new, narrow lines were observed as a result of the higher resolution. The coverage and resolution of this technique can be extended by using other metastable species (e.g.,  $\text{Li}^+$  or  $\text{Be}^{++}$ ) that have larger excitation energies and lower Doppler widths.

Both of these techniques produce bright, monochromatic, tunable, polarized radiation. Furthermore, the output follows the laser pulse in time, so that sub-picosecond pulses can be

produced. The light is spectrally narrow, and its frequency is accurately determined from the easily measured dye-laser frequencies. Thus the long-standing problem of accurately measuring a frequency in the VUV is overcome.

## **2. Precise Measurements of Line Positions and the Application to Time Standards**

Recent work in ultra-high precision spectroscopy is leading to improved accuracy in frequency determinations. Such improvements in turn lead to the need to refine the basic standard of time. Precision measurements of time and frequency have traditionally been connected with atomic spectroscopy, and the current definition of time is based upon an atomic measurement of the energy difference between two hyperfine levels of cesium. The current standard of time, defined only to a precision of about 1 part in  $10^{13}$ , lags significantly behind current capabilities for high precision frequency determination.

Prospects for new standards involve tunable laser light sources locked to the natural transition frequencies between quantum levels. The ability to compare oscillators of different frequencies is a necessary part of the precision time scheme, and it is now possible to compare frequencies over an enormous range from radio frequencies all the way to the optical regime. Particularly important to the frequency comparison chain is the use of non-linear optical mixing techniques.

The accuracy of time standards is compromised by the Doppler effect due to the relative motion between the quantum absorber and the laser oscillator. New sample preparation techniques include electromagnetic cooling of ions in traps and laser cooling of atoms in beams (Fig. 5). Workers using ion traps have cooled single ions and at the same time have recorded the spectrum of the ion. In due course, these impressive techniques will be coordinated into a new definition of time.

### 3. Ultra-Sensitive Probes of External Fields

Modern experiments use tunable lasers to excite atoms selectively to individual quantum states. Several techniques rely on the extraordinary sensitivity of highly excited atoms to their environment. The use of such atoms as sensitive probes of external forces has just begun to be explored. Atoms can be prepared in specific, highly excited (Rydberg) states and used as extremely sensitive detectors of weak external fields. In a typical experiment, an excited atom is ionized, before it decays by fluorescence, using a strong, applied dc electric field. Either ions or electrons are then detected with an efficiency near unity. Since each quantum state has a threshold for ionization at a well-defined and distinct field value, excited states may be identified by noting the applied field value at which ionization takes



**FIG. 5** Micro-photographic images of 1, 2, and 3 trapped  $\text{Ba}^+$  ions. The large photograph shows the  $\sim 2 \mu\text{m}$ -thick image (white arrow) of a single ion inside the rf quadrupole trap. The ion is made visible by laser-induced fluorescence. The view is taken through the gap between the ring and the left cap electrode (the trap structure is illuminated by scattered laser light). A reduced-scale sketch of the entire trap structure is shown at the upper left. The three small photos show, ten-fold enlarged, the central trap region containing 1, 2, and 3 ions, going from top to bottom respectively.

place. A recent study revealed the surprising result that Rydberg levels at an energy higher than that which was selectively excited were being populated because of the additional absorption of weak, room-temperature, blackbody radiation.

#### 4. Radiative Decay Rate Measurements

Because of the intrinsic difficulties of making the measurements, accurate transition rates (lifetimes, oscillator strengths, line strengths) are known for only a few simple atoms. Measurements of relative strengths by absorption, emission, and other techniques in neutral and singly ionized atoms have demonstrated uncertainties ranging from a few percent, in a few select cases, to 50% or worse. Lifetime measurements in more highly stripped ions have generally been made only by the beam-foil technique. Coherent excitation in the beam-foil interaction leads to quantum beats superposed on radiative decays. These beats provide accurate atomic structure measurements, as shown in the example of Fig. 6. Time-resolved fluorescence of atoms following selective population of individual energy levels can also provide accurate measurements of atomic lifetimes. The availability of new UV lasers will allow the extension of these techniques to lifetime and other time-dependent studies of most neutral atoms and, eventually, of ions. Ion storage with ion traps has recently provided a versatile technique for the direct, accurate measurement of the lifetimes of metastable and forbidden states of singly and multiply charged ions.

Two examples of laser excitation of fast ion beams show both the improved precision and the range of possible measurements. The decay times of the Li and Na resonance transitions, at  $14904\text{ cm}^{-1}$  and  $16973\text{ cm}^{-1}$ , respectively, have recently been measured to a precision of 0.2% in the geometry of a fast atomic beam excited in a small volume by a crossed laser beam. The fluorescent decay of the upper level was spatially resolved along the atomic beam path. The results represent at least an *order of magnitude improvement* in experimental precision over

previous methods and show the inadequacies of many theoretical approaches in treating even these simple systems.

Alternatively, collinear excitation of fast ions by lasers provides an enhanced reaction volume and increased efficiency. Time resolution may be achieved by rapidly shifting the laser frequency out of resonance. Applications to complicated spectra become feasible, as shown in recent lifetime measurements in  $\text{Er}^+$ .

### 5. Studies of Highly Stripped Atoms in Excited States

The development of light sources that are capable of producing atomic ions in extremely high stages of ionization has made it possible to observe spectra of ionization stages not previously attainable in the laboratory. Low inductance sparks, beam-foil excitation, and pinched discharges are examples of

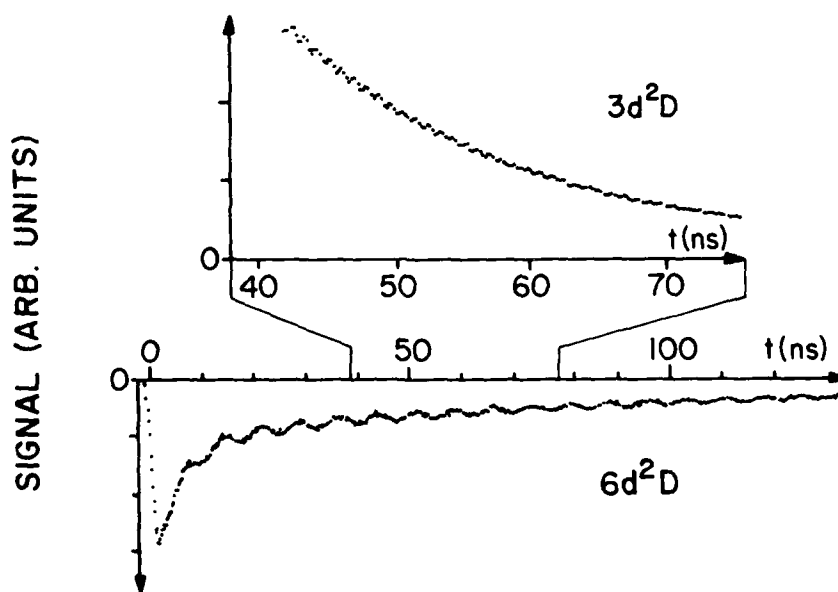


FIG. 6 Experimental fine structure, quantum-beat measurements of excited-state decay in  $\text{Li I}$ , following excitation by a beam-foil interaction. Depicted are quantum beats for the  $3d^2D$  and  $6d^2D$  terms.

such sources. A particularly desirable feature of these sources is their capability for preferentially exciting atoms to high stages of ionization to the relative exclusion of lower stages, thereby simplifying the interpretation of the spectra.

Spectra of highly ionized atoms (from  $\text{Sr}^{26+}$  through  $\text{Pd}^{35+}$ ), obtained with high power lasers, have recently been reported. The spectra in the region around 10 nm were found to be due almost entirely to simple ions isoelectronic with neutral Na and Mg. The identification of the  $4s^2 \ ^1S_0 - 4s4p \ ^1P_1^o$  resonance lines in  $\text{Zr}^{28+}$  and  $\text{Mo}^{30+}$  provides a basis for the use of these transitions in the diagnosis of hot plasmas found in tokamaks, which are themselves sources of information about highly ionized atoms. In other experiments with laser-produced plasmas, species as highly ionized as  $\text{W}^{45+}$  and  $\text{Au}^{51+}$  have been reported.

The development of high-resolution spectrographs in the soft x-ray region has greatly improved the quality of data for highly ionized species. For example, the use of such a spectrograph to observe spectra of the iron-like ions  $\text{Sr}^{12+}$  to  $\text{Mo}^{16+}$  has allowed a complex group of transitions to be analyzed and the energy levels determined.

Tokamak researchers have now observed magnetic dipole transitions at about  $20,000 \text{ cm}^{-1}$  within the ground configurations of  $\text{Zr}^{14+}$  and  $\text{Mo}^{16+}$ , providing accurate values for ground-term intervals in these ions. The long wavelengths (for such highly ionized species) of these lines place them in convenient spectral regions and make their Doppler widths easy to measure, thereby providing a monitor for ion temperatures in high-temperature, low-density plasmas.

The spectroscopy of highly ionized atoms plays a role in the effort to develop lasers operating in the soft x-ray region. For example, one technique being pursued is the creation of a population inversion by a two-step process in which the formation of a laser-produced plasma is followed by recombination into an excited state. A second technique involves the use of an intense Z-pinch to excite, *via* collisions, highly charged neon-like ions (such as  $\text{Kr}^{26+}$  or  $\text{Mo}^{32+}$ ) from the  $2p^6$  ground state to the

$2p^53p$  excited state, creating an inversion between the  $2p^53p$  and the  $2p^53s$  populations.

#### **6. Rapid Acquisition of Spectral Data by Fourier Spectroscopy**

The observation of low stages of ionization, traditionally carried out with grating spectrometers, has been revolutionized by the advent of Fourier transform spectroscopy (FTS). In this technique, radiation from a steady source is passed through a Michelson interferometer, the transmitted light is measured as the pathlength difference between the arms is varied, and the signal is relayed to a computer, where modern, fast Fourier transform techniques provide intensity vs. frequency over a large spectral region. Complete spectra may be obtained with a resolution as high as  $0.002\text{ cm}^{-1}$ , over a range of  $40000\text{ cm}^{-1}$ , in a total observing time of  $\sim 1$  hour.

With the present state of the art, the FTS can be used to record spectra between 200 and  $40000\text{ cm}^{-1}$ . Extension of the technique to higher frequencies is under way. Recent applications of FTS have included the observation of spectra of U and  $U^+$ , providing data critically needed for the efficient separation of uranium isotopes through the use of tunable lasers (see Chapter VI, Section B4).

#### **C. Spectroscopic Tools**

Current experimental techniques rely heavily on the experimental tools produced by modern technology. A discussion of the improvements anticipated and the problems to be solved for several such tools is now presented.

##### **1. Light Sources**

The use of storage rings and laser-generated plasmas as VUV light sources has opened up the study of transitions corresponding to core excited and multiply excited atomic systems. Synchrotron radiation from storage rings now provides an in-

tense source of calibrated, polarized radiation from the infrared through the soft x-ray region, and the introduction of wigglers and undulators should provide a major increase in intensity in the near future. In addition to new information on level positions, the combination of VUV excitation with electron energy analysis allows the various channels of excitation to be distinguished. A recently introduced technique, selective laser excitation of atoms, in a beam or a vapor, followed by short wavelength photoabsorption, has allowed exciting studies of the interaction between valence electrons and core electrons.

The broadband coverage of synchrotron radiation, vital to many studies, will be complemented by the higher intensities and spectral resolution of short wavelength lasers now in the development stage. Such sources could be used to produce even higher frequencies by nonlinear optical mixing processes. These nonlinear processes now employ sources below  $50,000\text{ cm}^{-1}$  because of a lack of sufficient intensity at higher frequencies.

Another important feature of coherent light generation is the capability of producing short pulses. Current techniques allow production of pulses of visible light as short as  $3 \times 10^{-14}$  sec, which represents about 15 optical cycles. With such a fast interaction time scale, we can measure lifetimes of autoionizing states, probe Rydberg states where the orbiting electron is effectively stationary during the pulse, create population inversions by ultrafast pumping, and study short-lived ground states of rare isotopes and nuclear isomeric or excited states.

## 2. Accelerators

The spectroscopy of highly stripped ions is intimately coupled to new sources now under development in various areas of physics and technology. Many new heavy ion accelerators will be completed and several others will be significantly upgraded in the next few years. These accelerators will provide significant quantities of most ions, up to and including uranium, at energies greater than  $10\text{ MeV/nucleon}$ , at velocities of at least a few percent of that of light. Several new ion sources have just

been developed that create highly charged ions at low velocities. The atomic spectroscopy of high-Z ions with only a few electrons will test calculations of QED and relativistic energy shifts. However, due to the low numbers of ions produced, experimental problems are anticipated with detecting the low photon flux, predominantly in the far-ultraviolet and x-ray regions.

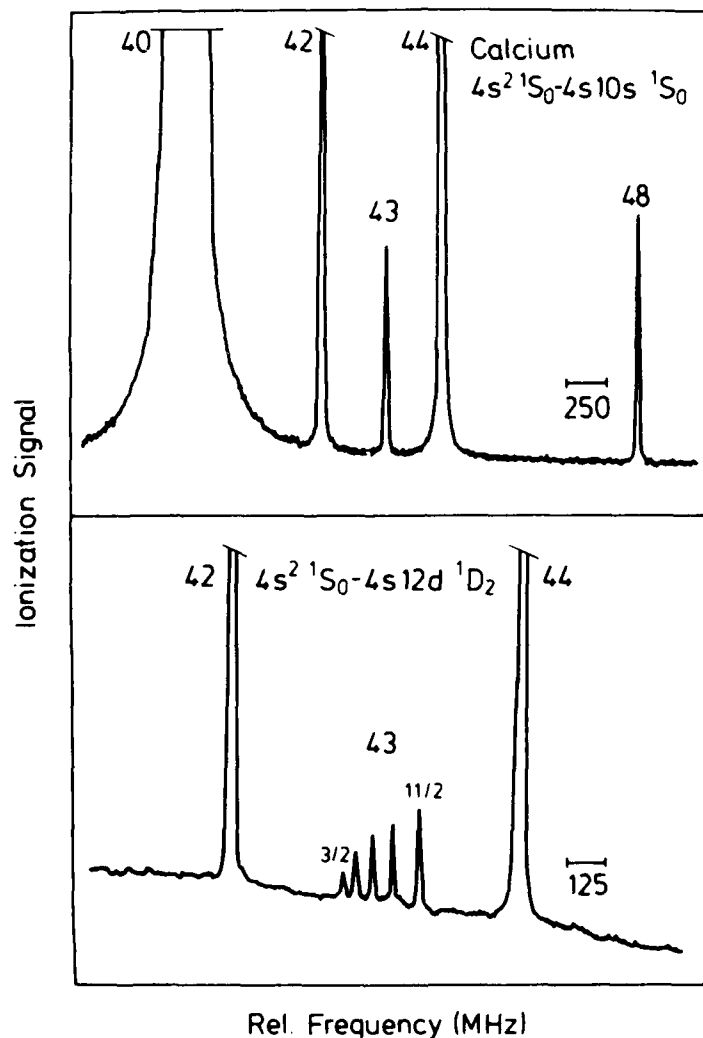
### **3. Gratings and Detectors**

The overall throughput and resolution of many spectroscopic instruments need to be improved. In grating spectrometry, diffraction grating efficiencies and resolution are a severe limitation on the performance of spectrometers. However, the introduction of blazed holographic gratings promises improvements in both spectral resolution and sensitivity.

Recent developments in UV photo-detectors promise to compensate for the low intensity of light reaching the detector. Many grating spectrometers are now being equipped with position-sensitive detectors (array detectors) in place of a scanning exit slit system. Single-photon detection with high spatial resolution (down to  $5\mu$ ), and with high spatial and intensity linearity, looks like an achievable goal in the near future. Many of these techniques are being pioneered by astronomers using, for example, charge-coupled device (CCD) arrays. Rapid data collection and analysis systems are needed to back up this new technology.

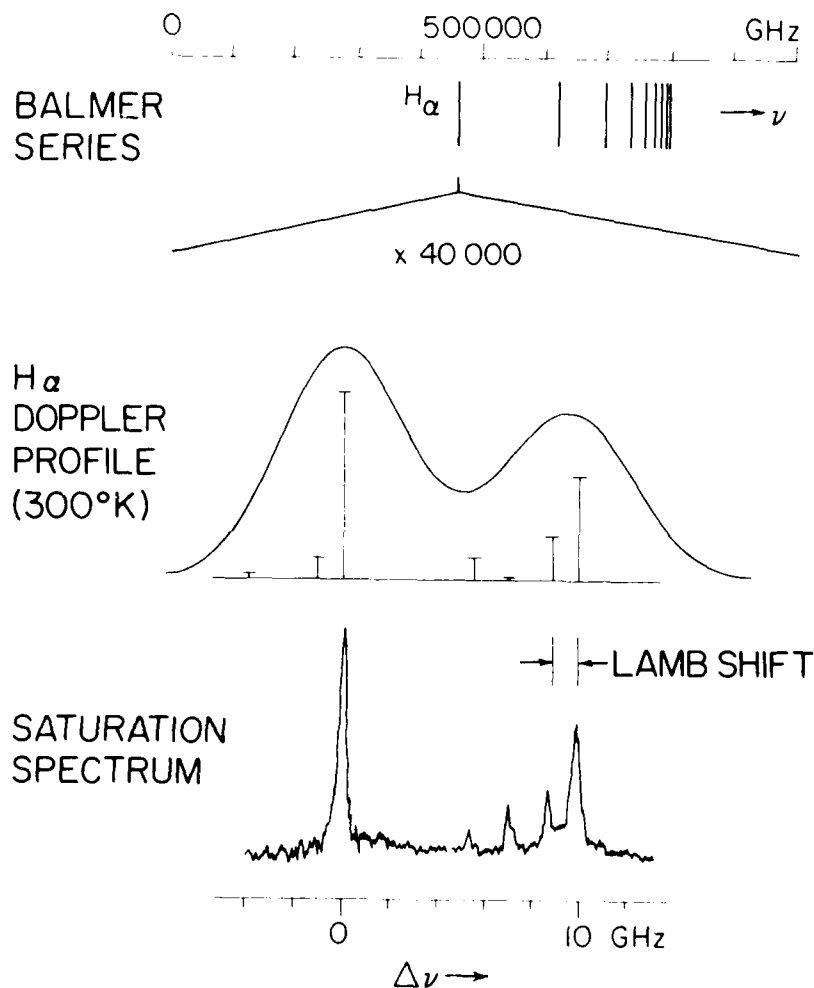
### **D. Spectroscopy for the 80's**

The past decade has been characterized by dramatic advances in both technology and concepts. The availability of tunable, coherent radiation from lasers has given rise to an exciting range of new techniques for measurements with high resolution, high precision, and high sensitivity. Two-photon absorption with counter-propagating beams and techniques using saturation of inhomogeneously broadened lines (saturation spectroscopy) remove Doppler broadening (see Figs. 7 and 8). The



**FIG. 7** Two-photon, Doppler-free, high-resolution excitation spectra of Ca I, recorded using a cw dye laser and thermionic diode detection. The biggest peaks extend off scale and are truncated for this figure. Upper trace: Well-resolved lines for different isotopes, corresponding to transitions from the  $4s^2\ ^1S_0$  ground state to the  $4s10s\ ^1S_0$  excited state. There is no hyperfine splitting because  $J=0$ . Lower trace: Well-resolved lines for different isotopes and hyperfine components, corresponding to transitions from the ground state to the  $4s12d\ ^1D_2$  state. Only  $^{43}\text{Ca}$  has a nuclear spin, and its effect on the  $^{11}\text{D}_2$  state is explained by singlet-triplet mixing - the observed hyperfine structure corresponds to a small admixture of triplet character into the singlet wavefunction. As a consequence, singlet-triplet mixing can be determined very precisely using hyperfine structure as the probe.

## SPECTRUM OF HYDROGEN



**FIG. 8** The Balmer  $\alpha$  line. Top: A schematic of a low-resolution spectrum of the Balmer series in hydrogen (transitions between  $n=2$  and  $n \geq 3$ ). Middle: The Balmer  $\alpha$  line (between  $n=2$  and  $n=3$ ), shown on a 40,000 times expanded scale, as seen in a hydrogen discharge tube at room temperature. The calculated intensities of the fine structure components are indicated by the bars. These components are smeared together by Doppler broadening due to the motion of the atoms in the discharge. Bottom: The resolved Balmer  $\alpha$  spectrum obtained using laser saturation spectroscopy to remove the Doppler broadening. The Lamb shift of the  $n=2$  states is now directly displayed in the visible region of the spectrum.

observation of polarization changes in transmitted beams (polarization spectroscopy) and the observation of intensity modulation when one sideband of a frequency-modulated beam is changed in intensity or phase (modulation spectroscopy) provide high sensitivity to absorption. The effect of laser probes on the current of hollow cathode discharges (optogalvanic spectroscopy) provides high sensitivity to transitions from excited levels in atoms and ions of refractory materials. Non-laser spectroscopy has advanced significantly with improvements in data acquisition techniques and different sources of excited atoms and highly stripped ions. Both laser and non-laser techniques will profit from the development of efficient mirrors, gratings and other coated optics in the far-UV and soft x-ray regions, as well as from the availability of new detectors and incoherent light sources such as synchrotron radiation. In general, we expect laser techniques to provide qualitatively new approaches to spectral studies, while conventional spectroscopy remains the major source of new data.

## V. COMPILATIONS AND TABULATIONS

### A. Introduction

Throughout all fields of science, a current trend is the establishment and maintenance of data banks containing refined, evaluated information representing the best values of the measurables of the field. Data compilations are an indispensable addition to the primary literature and, if they are to be useful to consumers whose expertise lies outside the field in question, must be prepared by experienced professionals. Critical data evaluation, a challenging and intellectually rewarding activity, immeasurably enhances the value of data compilations and provides a vital service to the community of users.

In atomic spectroscopy, these data banks include the frequencies, wavelengths, oscillator strengths, etc., that are either derived from laboratory measurements or calculated by various theoretical or empirical methods. Evaluated data impact the scientific community as follows: (1) the compilation process often reveals fundamental inconsistencies/conflicts in the data, (2) applied spectroscopists require a rapid means for obtaining reference data, (3) the compilations are a pathway to the literature wherein the best experimental and computational work is presented, (4) theoreticians depend on reliable data with which to compare their predictions and/or develop models of physical

processes, and (5) the compilations indicate the state of our knowledge of the data.

C. E. Moore's tables of atomic energy levels of the 1950 era are an outstanding example of spectroscopic compilation, and they have stimulated advances in every area touched upon by this report. In addition to showing the regularities and irregularities of the energy levels of atoms and ions, they reveal the incompleteness of each analysis and provide a jumping-off point for new experiment and analysis. Although Moore's tables are now about thirty years old, they are undoubtedly the most widely used source of atomic data today.

#### **B. Critical Data Compilation: Status and Needs**

A number of compilations of critically evaluated data exist, and others are in progress or are planned for the near future. For a listing of existing critical compilations and an indication of some of the critical data-evaluation projects in progress, see Appendix A.

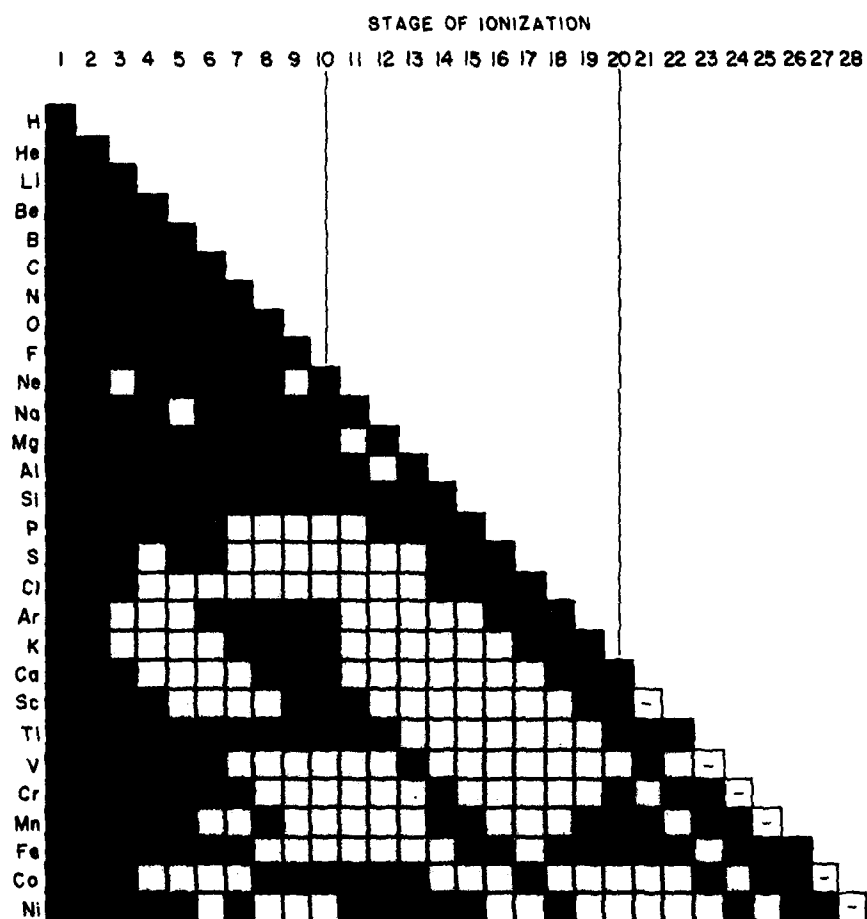
The data that are incorporated into these compilations vary widely in number and quality for the different quantities tabulated. In some cases the paucity of critically evaluated data is due to lack of research results in the primary literature, whereas in others it reflects the inadequacy of resources devoted to data evaluation/compilation efforts (i.e., in comparison to the more rapid growth of the primary data base).

Line position (equivalently, frequency, wavenumber, or wavelength) values are generally abundant and of high precision. They can be reduced to energies of specific quantum states of specific species when the spectral features from which they are derived can be identified as to atomic or ionic species and classified according to the upper and lower quantum states involved in the transitions. Line strength (equivalently, oscillator strength or transition probability) values are far less ubiquitous in the scientific literature, and uncertainties in many of the published values are at the 50% level or worse.

The current status of critically evaluated data on atomic energy levels and atomic transition probabilities for atoms from atomic number 1 (H) to 28 (Ni), for all stages of ionization, is summarized in Figs. 9 and 10. The classification of spectral lines and quantification of energy levels, derived from analysis of experimental spectra, are extensive, but are generally characterized by decreasing availability and accuracy with increasing atomic number or stage of ionization (Fig. 9). The data on oscillator strengths, which for ions beyond the second stage of ionization are derived primarily from theoretical calculations, are generally far less complete and less accurate than energy level data, with the exception of the hydrogenic spectra (Fig. 10).

Several compilations of atomic wavelengths are available, some of which are quite extensive in terms of coverage of the electromagnetic spectrum and/or atomic/ionic species. These are usually arranged in one of two principal schemes: (1) ordered primarily by spectrum (i.e., element and stage of ionization), and secondarily by wavelength; (2) ordered by wavelength, regardless of spectrum. (This latter arrangement is known as a "finding list," and it enables the user to identify the spectrum to which a particular spectral feature belongs, given its wavelength.) Coverage is quite good for wavelengths in the visible, ultraviolet, and near-infrared regions of the spectrum. More work is needed, however, in the x-ray and far-infrared regions.

Some compilations of ionization limits and ionization potentials are available, and these quantities are often included in compendia of wavelengths or energy levels as well. Tabulations of critically reviewed data on Stark widths and shifts are available but cover a very limited number of spectral lines. Lifetimes of excited atomic and ionic states have not been critically compiled on a large scale, but they do figure in the critical evaluation of atomic transition-probability data in that they are often utilized to determine an absolute scale to which relative values can be normalized. More compendia, in tabular or graphical form, of evaluated data on photoabsorption and photoionization cross sections are needed, as are tabulations of hyperfine



STATUS OF ANALYSIS OF ATOMIC SPECTRA

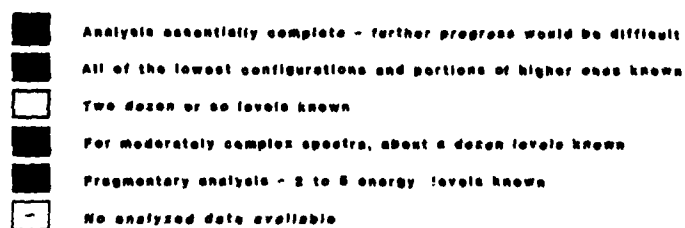
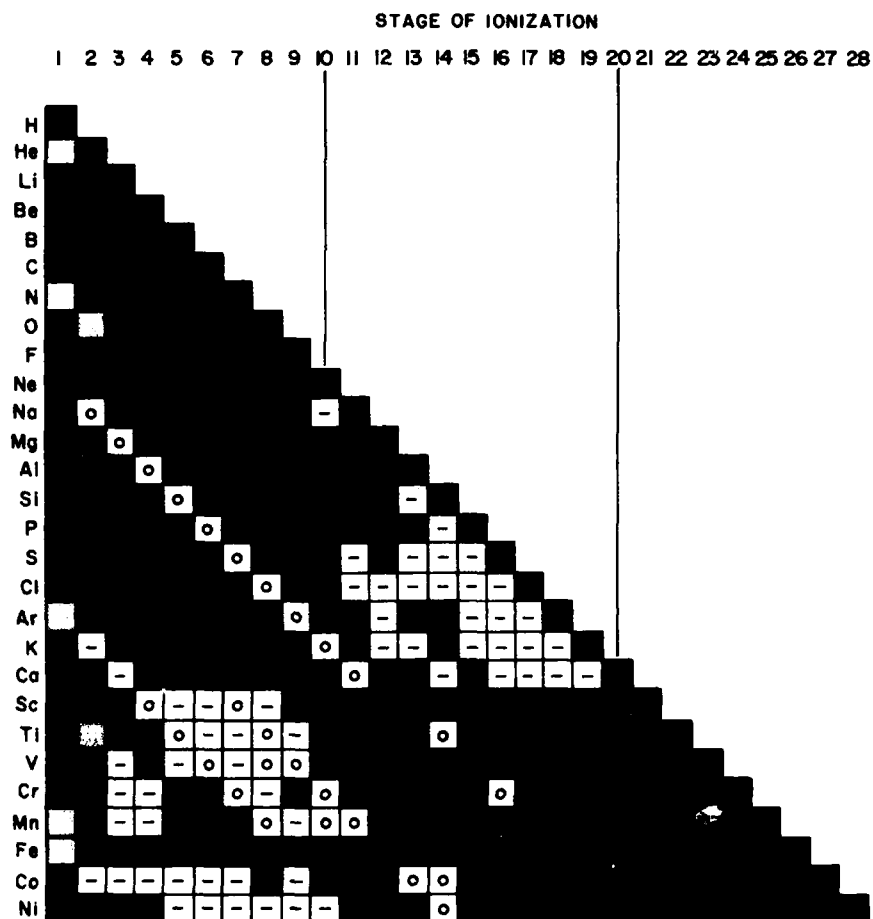


FIG. 9



### EVALUATED OSCILLATOR STRENGTH DATA

- Hydrogenic spectra. Oscillator strengths are accurately calculated from wavefunctions
- Data of relatively high accuracy are reasonably abundant
- A fair number of relatively high accuracy data or a large number of moderately accurate data are available
- Either a small number of high accuracy or a large number of low accuracy
- Low accuracy data for a few transitions
- No evaluated data available

FIG. 10

structure. Also, the advent of experimental techniques that enable researchers to probe high-lying Rydberg levels, as well as doubly or multiply excited states, has created a need for critically evaluated spectroscopic data that pertain to such studies.

Structural parameters that are the results of *ab initio* or semiempirical calculations have appeared in the primary literature, but critically evaluated tabulations are practically nonexistent. These parameters quantify in some way the atomic wavefunctions, the expectation values of dynamical variables, and the contributions of various electromagnetic interactions to the energy-level structure of atoms and ions. Since a relatively small number of such parameters can be used to construct, say, an entire energy-level spectrum, and since the values of the parameters are, in general, highly dependent on the theoretical model used to derive them, it is important that they be subjected to critical evaluation.

### C. Routes to Data

There are a number of centers that are dedicated to the critical evaluation and compilation of atomic spectroscopic data, as well as to the collection and cataloging of literature references, maintenance of a master reference list, and in some cases publication of bibliographies. A listing of pertinent information concerning locations of these centers, scope of collection, names of individuals to whom inquiries may be directed, and services provided can be found in Appendix B.

In addition to critically evaluated data, a number of extensive tabulations of the results of theoretical calculations and/or experimental investigations are available, but should be used with some caution if they have not been subjected to the critical-evaluation process. Examples of journals in which tabulations of atomic data are likely to be found are the following: *Atomic Data and Nuclear Data Tables*, *Astrophysical Journal Supplement Series*, *Astronomy and Astrophysics Supplement Series*.

In the absence of existing data compilations or large tabulations of high-quality data, bibliographies serve to direct

the user to the pertinent sources of data in the primary literature. To the extent to which these bibliographies classify references according to species, atomic quantities treated, method used to derive the results, etc., a search for information or data can be narrowed rather substantially with little effort, thus eliminating the need for the user to conduct his/her own search from scratch. Compilers of bibliographies can further narrow the set of literature references that a potential user would have to consult, by being selective in choosing references for inclusion in a bibliography. This selection process is best undertaken after a critical evaluation/compilation of the data has been done, since experienced data evaluators are in an ideal position to make such judgments. A list of published bibliographies is given in Appendix C. References that have appeared in the literature subsequently to the most recently published bibliographies are often available from the data centers or individuals who prepared them.

An additional route by which users of data may become aware of existing and soon-to-be-published data compilations as well as primary data sources is *via* newsletters. Such instruments serve to disseminate information in a timely fashion and to promote communication among producers, evaluators, and end users of information and data. They also have the potential for facilitating the exchange of computer programs (e.g., a program that computes all possible transitions for a given spectrum, given the list of known energies along with their quantum numbers) and/or stored data on tapes or disks. A listing of newsletters that are currently in circulation can be found in Appendix D. However, a more general newsletter is needed, covering the literature (and work in progress) on a wider range of atomic spectroscopic quantities and unrestricted in terms of atomic or ionic species, in contrast to existing newsletters that address the needs of specific user groups.

#### D. Computer Data Bases

A major problem associated with modern data compilations is that of making the information readily accessible. Recourse to highly automated procedures is inevitable and essential for speed as well as convenience. Information centers will therefore establish data base management systems and facilitate access to them. Consider, for example, the following scenario. Since the necessary hardware is already available and there are no *technological* roadblocks to immediate implementation, it could take place in the near future:

*An astronomer needs a list of Al II lines for which moderately accurate gf-values are available. He turns on his office terminal, dials a local number, and connects his modem. After a few simple commands he is signed onto the computer of the ATOMIC DATA CENTER several thousand miles away. He issues a RUN command to start a program that will give him access to the CENTER's atomic data base. In a few moments he responds to the interactive program's first query, which asks whether the information desired concerns properties of atomic states or properties of transitions. He enters a "T" for transitions and sees the response "ENTER THE CHEMICAL SYMBOL FOR THE ELEMENT." After typing "Al" and then "2" for the second spectrum (singly ionized aluminum), he responds to further prompts to restrict the search by wavelength, excitation energy, and oscillator strength. At this point, a search is performed and the desired information is written into a temporary file at the CENTER'S computer. More options appear, giving a choice of methods of retrieving the data. Moderate amounts of data can be telecopied directly to the disks of the user's home computer, while larger amounts will require special high transmission rates. Our user wants the data records for only the stronger Al II lines with oscillator strengths of uncertainty 25% or better. He copies them to his local disk and signs off.*

Several groups, both in the U.S. and elsewhere, are beginning to set up computer-based atomic physics data banks. The payoff from such efforts will be immediate in fields such as

astrophysics and plasma diagnostics, where calculations will be facilitated as soon as such data bases become available. In developing a computerized data base, both the data center and the user community should be involved in studying the potential form and content of the design, so that a useful, high-quality system is produced. Once the data base is established, documentation should be available both on-line and through the mail, and run-time information should be available through a HELP command.

It must be emphasized that the computer can only *speed* the management, display, and exchange of information. The *quality* and *utility* of the data will *still* depend upon the concentrated efforts of trained professionals who evaluate and prepare information for entry in the data base. The timeliness of their efforts is enhanced by computers, but in no way do computers replace these specialists.

#### **E. Critical Factors to be Considered in Evaluation of Data**

The manner in which researchers report their results and the format of the results have the potential for influencing the quantity and the quality of data that are selected for inclusion in critical compilations. The extent to which certain "critical factors" have been considered in performing the experiment or in carrying out the calculations, as well as the degree of clarity and completeness with which this information is reported, is very important to data evaluators. Some examples of critical factors are the following:

1. An investigator who publishes classifications of spectral features should be explicit concerning the evidence used to arrive at the classifications.
2. Theorists should provide an explicit list of configurations (or channels) that were included in the calculations. They should publish eigenvector components, including phases, and a clear definition of the phase convention that was used.

3. Experimentalists who produce data on strengths of spectral features should indicate whether, and to what degree, effects such as self-absorption, line blending, background corrections, etc., affected the results.

4. There should be considerable emphasis placed on the discussion of random and systematic errors.

The evaluators themselves have certain obligations. For example, uncertainty estimates should accompany the compiled data, and the precision of the tabulated numerical values should be commensurate with the estimated uncertainties. All sources of compiled data should be mentioned, and at least a short text should be included to document and describe the data selection.

## **VI. APPLICATIONS OF ATOMIC SPECTROSCOPY**

### **A. Introduction**

Advances in the field of atomic spectroscopy have had and will continue to have significant impact on progress in other fields of science, areas of modern technology, and society in general. In this section we discuss some specific examples of how atomic spectroscopy is applied to problems outside of traditional atomic physics. We provide examples where progress in areas distinct from atomic spectroscopy as well as at the diffuse border (see Chapter I, Section D) is closely tied to improvements in experimental spectroscopic techniques and to improved theoretical understanding of spectroscopic data. Because of these close ties, there is a great demand for more precise values of energy levels and oscillator strengths and for a deeper understanding of, and further data on, basic atomic processes such as photoionization, recombination, collisional interactions, multi-photon excitation, etc. With the advent of a large assortment of new coherent and incoherent light sources and new experimental techniques, atomic spectroscopists are supplying information of unrivaled precision and scope in these areas.

In the following paragraphs we discuss a few highlights out of the vast number of applications of atomic spectroscopy

and try to indicate the many fertile areas that are sure to bear fruit in the next few years.

## **B. Highlights**

### **1. Fundamental Physics and Precise Measurements**

Since the techniques of spectroscopy are the most precise in all of measurement science, it is natural to apply them to both of the nearly inseparable endeavors of testing fundamental physical ideas and establishing measurement standards.

Atomic spectroscopists provided the first experimental challenges to the classical understanding of particle dynamics and thus helped usher in the quantum era of today. Progressively more precise experiments on atomic fine structure have led to the development of relativistic quantum theory, the discovery of particle spins, the discovery of the anomalous magnetic moment of the electron and the Lamb shift, and the development of modern quantum electrodynamics (QED). Most of these advances in our understanding of microscopic particle dynamics were catalyzed by *unprecedented improvements in experimental resolution and accuracy*. Now, the generally comfortable mutual agreement between fundamental atomic experiment and theory is likely to be disturbed again shortly by striking advances in the traditional testing grounds of atomic spectra, namely two- and three-particle atoms.

One example is provided by the observation of two-photon, Doppler-free spectra of the 1s-2s hydrogen transition. These measurements offer the potential for greatly improved accuracy of determining the 1s Lamb shift with an inherent natural precision a thousand-fold better than the originally discovered 2s Lamb shift. By incorporating direct optical metrology, one could conceivably improve the accuracy another factor of ten thousand, limited by the present measurement standards. Ultimately, another factor of 100 improvement, limited only by the 1 Hz natural linewidth of the 2s state, is possible.

Another example is the long-awaited observation of the 1s-2s positronium (Ps) transition. This experiment has the potential for a thousand-fold resolution improvement in the measurement of the Lamb-shift in a *purely leptonic system*, a system free from the theoretically troubling nuclear size effects. Precise laser spectroscopy of this and other exotic atoms, such as the muonium systems, can be expected to provide some of the most rigorous tests of QED.

Three-particle systems are similarly candidates for precise tests of quantum-theory formulations and still speculative, long-range, many-body interactions. This class contains several examples of both normal and exotic atoms, such as  $\text{H}^-$  ( $e^-p^+e^-$ ), helium ( $e^-\alpha^+2e^-$ ), muonic helium ( $\mu^-\alpha^+2e^-$ ), and  $\text{Ps}^-$  ( $e^-e^+e^-$ ). The considerable body of sub-natural-linewidth spectroscopic data on helium already presents a challenge to theorists.

To carry out many of these fundamental measurements, instrumental resolution must be further improved. The theoretical limiting linewidths of lasers are in the mHz range, and rapid progress in stabilization, noise reduction, and calibration is being made in several laboratories. Linewidths of a few Hz, stable over many seconds, have been observed. The primary sources of sample broadening are collisions, external field perturbations, Doppler shifts, transit-time effects, and photon-momentum recoil. As an example of successful reduction of these effects, a single ion may be isolated in a trap (Fig. 5), radiatively cooled, and stored for hours at a kinetic temperature of a few milliKelvin. Recoil may be eliminated by simultaneous absorption of multiple quanta whose momenta sum to zero. With these techniques, microwave linewidths of  $\sim 10^{-3}$  Hz have been observed. If one could reach these natural resolution limits, one could test in a *few days' time* Dirac's speculation that fundamental constants vary with the age of the universe. This could be done by comparing the frequencies of two spectral lines whose dependence on fundamental constants is different, such as lines containing atomic fine- and hyperfine-structure levels.

It is important to note the symbiotic relationship between high-resolution experiments and the development of better measurement standards. For example, the length standard is now proposed to be redefined in terms of the currently accepted time standard (the cesium clock) and the speed of light, which would be fixed at 299,792,458 m/s exactly. The frequency and wavelength calibrations required to establish the connection between the length and time scales throughout the electromagnetic spectrum will be done spectroscopically using the techniques employed in the experiments mentioned above.

The recent progress in laser spectroscopy and metrology has spurred interest in their use in astrophysics and geophysics. For example, subnanosecond pulsed lasers and accurate atomic timing methods have allowed measurement of the earth-moon distance with an accuracy of a few centimeters. Frequency-stabilized lasers and interferometric techniques have been used to measure the acceleration of gravity to 9-digit accuracy. Recent progress in frequency-stabilized lasers should allow detection of length changes as small as  $10^{-15}$  cm, much smaller than a typical nuclear dimension. There is a significant effort worldwide in applying these laser techniques to the search for gravity waves using long baseline interferometers as gravitational antennas.

## **2. The Generation of Coherent Light**

The development of coherent sources at wavelengths not currently available - in the ultraviolet (UV), vacuum ultraviolet (VUV), and shorter, and in the infrared (IR) - can benefit significantly from an increased data base of atomic spectroscopic information. For example, there are many potential short-wavelength-laser schemes, particularly in higher stages of ionization, in which both modeling and experiments cannot even begin until further spectroscopic data are obtained.

The generation of coherent light made its first major appearance in 1960 with the discovery of the laser. In addition to the laser being the light source that has revitalized atomic

spectroscopy as well as many other areas of science, it has found widespread use in such diverse areas as surgery, lithography, printing, welding, machining, construction, communications, and remote sensing. The discovery of new lasers would have been difficult, if not impossible, without the detailed knowledge of energy levels, oscillator strengths, and other basic parameters derived from atomic, molecular, and solid state spectra. The first laser, operating in a ruby crystal, is a prime example. Chromium ions were found to retain their atomic characteristics when imbedded in solid matrices such as sapphire ( $\text{Al}_2\text{O}_3$ ). Knowledge of Cr ion spectra was essential in formulating the laser model. The discovery of the first gas laser - the helium-neon laser - was also made possible by the availability of relevant atomic spectroscopic data. The development of most other lasers, including the argon ion laser, one of the workhorses of tunable laser spectroscopy, has similarly benefited from knowledge of such data.

Frequency multiplication and down-conversion of light from laser sources have allowed access to wavelengths that were unobtainable with lasers themselves (see Chapter IV, Section B1). The use of atomic vapors in obtaining efficient frequency conversion by phasematching was made possible by the knowledge of the index of refraction of various gases and metal vapors at a wide range of wavelengths, which in turn required knowledge of atomic energy levels and oscillator strengths.

The ready availability of atomic spectroscopic data, coupled with other technical expertise in visible optics, has made the visible region the playground for laser developers. Other spectral regions are hurting for lack of such information. In the ultraviolet, there are a few lasers, such as the highly efficient excimer lasers, that provide high pulse powers at several wavelengths, but these lasers are relatively expensive, lack narrow-line features and tunability, and are limited to relatively short pulse lengths. The shortest wavelength, commercially available, cw laser is the HeCd laser at 325 nm. Below 190 nm, only a few lasers have been discovered, and these are still, for the most part, laboratory curiosities. At less than 110 nm, the only co-

herent sources are obtained from frequency multiplication of UV, visible and near-IR lasers, using processes that are presently quite inefficient. The same story is applicable to the IR. Except for several examples, such as the CO<sub>2</sub> laser, there are many large gaps in the available spectrum of useful laser sources.

In seeking shorter-wavelength lasers, higher stages of ionization of atoms must be accessed. In many instances the atomic parameters are not yet known for the species that could become the best laser candidates. The most efficient excitation and ionizing techniques have yet to be determined.

### **3. Surface Science and Microelectronics Technology**

Both surface science and microelectronics technology are just beginning to be investigated by atomic spectroscopic techniques. New and exciting surface science studies feature the spectroscopic investigation of atoms in positions adjacent to surfaces. Similarly, the dry processing techniques used extensively in microelectronic circuit fabrication are now being studied by means of such spectroscopic investigations. This parallel development is appropriate, since one of the chief motivations for the study of surface science is the dependence of microelectronics technology on the interaction between solid surfaces and gases. Microelectronics chips are fabricated by a series of dry processing steps (e.g., etching, oxidation, doping of semiconductors, deposition) involving gases, plasmas, and atomic ion beams interacting with solid surfaces.

Spectroscopic techniques are also being applied to the observation of atoms and atomic ions impinging on and/or leaving a surface. One class of surface science investigations features the deposition of energy on a surface and the study of atoms leaving the surface. Techniques such as sputtering by (fast) ion impact, (fast) electron-stimulated desorption, (VUV and soft x-ray) photon-stimulated desorption, and thermal-induced desorption yield atoms in the ground and excited states. Highly sensitive state- and species-selective laser spectroscopic

techniques such as induced fluorescence, absorption, and ionization will yield valuable information about these processes. For microelectronics fabrication techniques, the science underlying the various dry processes can be addressed by these same laser-spectroscopic investigations.

The successful implementation of these techniques depends on the availability of spectroscopic data for many atoms and ions. For example, improvements in microelectronics technology demand improved etching techniques. An etching method much in vogue is known as reactive ion etching (RIE). In RIE, the substrate (to be etched) lies on an electrode through which rf power is coupled to a gas mixture, generating a plasma. The electrode becomes negatively charged relative to the plasma, causing positive ions to be accelerated toward the substrate. The ions as well as un-ionized atoms, molecules, and radicals in the plasma react with the substrate, leading to etching that may be highly directional and/or highly selective. The etching rate is strongly enhanced because the various species in the plasma are produced in excited electronic states, leading to increased chemical reactivity. The study (and process monitoring) of RIE by laser spectroscopy will depend on data, not currently available, on atomic species such as C, F,  $F^+$ , Al,  $Al^+$ , Si,  $Si^+$ , Cl,  $Cl^+$ , Ti, and Cu (as well as on molecules and radicals), important constituents of various RIE plasma-substrate systems.

#### **4. Selective Photoionization - Laser Isotope Enrichment and Mass Spectrometry**

Sequential, multiple-photon excitation experiments have demonstrated the ability to selectively ionize and detect *a single atom* in the midst of more than an atmosphere's pressure of other atoms and molecules. An increase in our knowledge of multiphoton ionization cross sections of atoms will lead to significant improvement in the efficiency of such multiphoton photoionization schemes for isotope enrichment and resonance-ionization mass spectrometry. The importance of laser isotope separation for uranium and plutonium is self-evident. Element-

selective, resonance-ionization mass spectrometry is becoming an increasingly important tool for the removal of isobaric (i.e., isotopes of different elements that have the same mass) interferences in mass spectrometric analysis. These isobaric interferences are currently removed chemically, and in many cases the elemental separation is inadequate.

A detailed understanding of the structure of the atom is the starting point for all photoionization schemes. Parameters such as energy levels, absorption cross sections, isotope splittings, hyperfine structure, lifetimes and branching ratios, and field and collisional ionization rates from Rydberg states are vital to the design of the multistep excitation scheme. Autoionizing states play an important role, but their positions and excitation cross sections are often unknown and difficult to calculate. The need for more data is evident from the fact that in the half-dozen atoms studied, approximately 30% of the observed resonances are not readily assignable to a known energy-level sequence. These unassigned resonances are often the most intense.

As an example of the leverage spectroscopy has on the economics of laser isotope enrichment of uranium, consider that lasers constitute a significant fraction of the projected cost of the process. If an ionization sequence could be found that has a 10% increase in cross sections over the present sequence, a savings of many tens of millions of dollars over the operation period of the separation plant would result.

## **5. Atomic Analysis - Complex Environments**

It is often necessary to determine concentrations of atomic species in a complex environment. These measurements are limited by our knowledge of interactions between the atom and its environment. Examples of complex environments include plasmas, flames, combustion engines, and high-pressure and/or high-temperature reactors. In addition to the data needed for the ideal, non-interacting system, information on pressure broadening, Doppler broadening, reactive and non-reactive

quenching, energy transfer, Stark broadening (both from the local environment and from the laser field) and the influence of high magnetic fields is necessary.

For example, laser-enhanced ionization in flames is the most sensitive method for the detection of many atomic species. The sensitivity of the process depends strongly on the properties of the energy levels coupled by the laser radiation. The important criteria include the closeness of the final state to the ionization continuum, the population of the initial state, collisional ionization rates, quenching constants, etc. In practice, the best (lowest detection limit) irradiation scheme has been found empirically. A deeper understanding of the system may lead to a more sensitive scheme.

Another new and sensitive technique for trace element detection involves focusing a laser to a small volume within a gaseous sample and monitoring the emission from the resulting spark. This technique has proved useful for environmental monitoring of trace concentrations of toxic elements such as beryllium. However, the strong electric fields formed by the focused laser cause shifts and splittings in emission lines and changes in quenching constants, which complicate the analysis. These complexities are currently being handled empirically. Once again, a more detailed understanding of the environmental interactions would lead to better analysis.

## **6. Nuclear Physics**

Atomic spectroscopy has been an important tool for the investigation of nuclear structure since the earliest days of nuclear physics. Data on nuclear spins and moments from atomic-beam magnetic-resonance experiments, as well as knowledge of optical hyperfine structure, helped to establish the nuclear shell model. The first evidence for the tensor nature of nuclear forces came from the discovery of the quadrupole moment of the deuteron. Systematic studies of isotope shifts in a given element have revealed remarkable, discontinuous changes in the rate of growth of the nuclear radius with neutron number.

The availability of tunable lasers has greatly increased the power of atomic spectroscopy to contribute to studies of nuclear structure (see Fig. 7). Very short-lived nuclei can be oriented by laser optical pumping of an appropriate atom or ion, and the resulting orientation can be detected by anisotropies in the nuclear decay radiation. Optical spectroscopic techniques - for example, the absorption of a laser photon by the isotopically shifted resonance line of a radioactive nucleus - can be used to control the angular distribution of much more energetic gamma rays or beta particles, thereby permitting the detection of very small numbers of atoms which could not be investigated by nuclear or atomic spectroscopy alone.

Spectroscopic studies of the hyperfine structure of rare isotopes can provide structural information on nuclei far from stability, i.e., nuclei that have many more protons or neutrons than do stable nuclei. These nuclei may have properties quite different from nuclei thus far studied. Once such new nuclei are discovered, some of the first properties of interest are the radius, spin, magnetic moment, and quadrupole moment. Given the small quantities of very short-lived nuclei that are produced with particle accelerators, the only known method of measuring most of these properties is that of high-resolution laser spectroscopy.

Atomic spectroscopic methods are widely used to produce polarized nuclei or electrons for particle accelerators. Lamb-shift sources, Stern-Gerlach magnets, and various optically pumped sources are all of use. Very intense sources of polarized tritons and deuterons may be produced by laser pumping of appropriate atoms, and these are being considered for enhancing the fusion rates in tokamaks and other magnetic confinement devices. Similar laser optical pumping methods are being developed to produce dense targets of polarized nuclei. The search for weak intranuclear interactions that violate fundamental conservation laws, like parity, time reversal, or charge conjugation, is being carried out with spin-polarized nuclei that have been produced by some of these spectroscopic techniques.

Nuclear physicists are rapidly developing experimental techniques to enable the study of the optical spectra of short-

lived isotopes. In one technique, a mass separator, on-line with an accelerator, provides a beam of radioactive atoms that interacts with light from a tunable cw dye laser. In such studies, a major limitation is the availability of cw single-frequency lasers in the ultraviolet spectral region.

## **7. Astrophysics**

Astrophysics rests on the interpretation of radiation reaching the earth, and most of our knowledge of the elemental composition, ionization state, temperature, and density of the atmospheres of stars and of interstellar matter has relied on detailed application of information derived from atomic spectroscopy. Rapid advances in the sensitivity, resolution, and wavelength range of astronomical observation demand more extensive and more precise spectroscopic data. There is a continuing need for a very large number of transition frequencies and oscillator strengths for analysis of spectra of the sun and all but the hottest stars. Such analyses of elemental abundances form the basis for the study of the creation, out of hydrogen, of all the other elements, a key part of our understanding of the evolution of the universe.

Models of radiation from stellar atmospheres may now be synthesized from over a million spectral lines. Such models reproduce many of the general features of high-resolution spectra, but even a casual comparison shows that many strong lines have not been included in the models. Since incompletely resolved features must be accounted for in the interpretation of the known spectral lines, and since the opacity of unknown lines clearly affects the observed spectral structure, extensive improvements in the completeness and accuracy of the atomic data are needed. For normal stars, more extensive analysis, especially in the UV, of the iron group elements is most important. Chemically peculiar stars require additional data on several stages of ionization of the rare earth and other heavy elements.

Extension of astronomical observations into the IR, UV, and x-ray regions has placed new demands on atomic spectros-

copists. This trend is sure to continue with the launch of the Space Telescope and other satellites. New possibilities will arise for the detailed study of physical environments in the outer envelopes of stars, the dark, interstellar clouds where star formation is in progress, and the nuclei of active galaxies and quasars. A striking example is provided by the recent discovery of solar emission lines near  $12\mu\text{m}$ . These lines have been identified as due to transitions between low-lying Rydberg states of Mg. The Zeeman splitting of these lines provides an outstanding tool for the study of magnetic fields in the sun and other stars.

There is generally a need to determine the densities and temperatures of *astrophysical plasmas*. For example, solar flare studies require these parameters in order to investigate the mechanisms for energy release. Observations are often limited to relatively strong emission or absorption lines, which generally restricts the analysis to the ten or fifteen most abundant elements. Since these plasmas are typically far from thermal equilibrium, models of the emitting regions require, for example, photoionization cross sections, collisional ionization and excitation rates, charge transfer rates, and radiative and dielectronic recombination rates. Intensity ratios are especially valuable to diagnose density or temperature when accurate transition probabilities and collisional cross sections are available. There has been immense progress in this area in the past few years, especially for line ratios at UV and x-ray wavelengths. Higher sensitivity and spectral resolution are making it possible to use line ratios involving weaker lines whose ratios vary more dramatically with plasma parameters.

## 8. Plasma Physics

Thermonuclear fusion in a plasma requires that high temperatures and densities be maintained as long as possible. Energy losses due to radiation by impurity ions must be minimized. Electron and ion temperatures and densities must be studied throughout the plasma to assess the effectiveness of confinement and heating techniques. X-ray spectroscopy identi-

fies impurities and provides accurate diagnostic tools for density and temperature. The important spectral lines and intensity ratios are the same as those encountered in solar flares, except that common impurity elements replace astrophysically abundant ones.

Density-diagnostic line ratios require metastable levels whose lifetimes are comparable to the collisional de-excitation rates. Iron ions in the boron through fluorine isoelectronic sequences have several appropriate levels. Helium-like ions are also useful because they exhibit strong lines. The O VII lines are appropriate at solar flare densities, and more highly charged ions would be suitable for the higher densities found in tokamaks. Knowledge of collisional excitation rates for these metastable levels has recently been improved by detailed calculation of the contribution of resonances.

Excellent temperature diagnostics have been developed using satellite lines. These are weaker lines at slightly longer wavelengths than a strong resonance line. Some are formed by dielectronic recombination and others by inner-shell excitation. The former measure electron temperature and may eventually measure the electron distribution function at discrete energies. The latter measure the ionization state of the plasma.

Models of the ionization distribution of an impurity element from the walls to the center of the plasma can be constructed from ionization rates and radiative and dielectronic recombination rates using densities and temperatures derived from these diagnostics. Comparison of the models with line intensity distributions can be used to study transport of ions in the plasma.

The electron and ion temperatures in a plasma can be quite different. Forbidden lines at ultraviolet wavelengths are advantageous for investigation of the ion temperature through measurement of the Doppler width.

While the spectroscopic study of plasmas requires a detailed knowledge of energy levels, transition probabilities, and collision cross sections, it yields a large amount of this information in return.

### **C. Summary**

Several areas where atomic spectroscopic data are needed have been highlighted. These data include energy levels, transition probabilities, collision properties, recombination rates, and the effects of strong electric and magnetic fields. The types of data needed in particular applied areas are shown in Table I. The data needs in areas of societal impact are shown in Table II.

In some cases, the data needed already exist but are hidden in the literature. In other cases, additional measurements are required. The need for better and more complete compilations is obvious. Consideration of transitions between excited states as well as from excited states into the ionization continuum is important. It is important to notice that a broad range of data is needed, and these needs are continually changing. It is often difficult to anticipate exact needs, yet the data should be available when the need arises. Often, costly delays in important projects occur while the needed data are being acquired, or, alternatively, non-optimal systems are used out of necessity or ignorance.

TECHNICAL FIELDS DATA										
	Fundamental Physics	Coherent Light Generation	Surface Science	Microelectronics Technology	Laser Isotope Separation	Atomic Analysis	Solar & Astrophysics	Plasma Diagnostics	Nuclear Physics	Solid State Physics
Line Positions	●	●	●	●	●	●	●	●	●	●
Line Strengths	●	●	●	●	●	●	●	●	●	●
Line Shapes	●	●			●	●	●	●		●
Energy Levels	●	●	●	●	●	●	●	●	●	●
Lifetimes	●	●	●	●	●	●	●	●		
Ionization Limits	●	●	●	●	●	●	●	●	●	●
Photoionization Cross Sections	●	●	●	●	●	●	●	●		●
Multiphoton Cross Sections	●	●		●	●	●				
Recombination Rates		●			●	●	●	●		
Isotope Shifts	●	●			●	●	●	●	●	
Hyperfine Splittings	●	●			●	●			●	
External Field Effects	●	●			●	●	●	●		●
Collisional Properties		●	●	●	●	●	●	●		●

TABLE I: DATA NEEDS OF VARIOUS AREAS OF SCIENCE AND TECHNOLOGY

AREAS OF SOCIETY  DATA	Physical Sciences	Industry	National Defense	Environmental Studies	Energy Sources & Utilization	Biomedicine	Metrology and Fundamental Constants	New Sources of Light
Line Positions	●	●	●	●	●	●	●	●
Line Strengths	●	●	●	●	●	●	●	●
Line Shapes	●	●	●	●	●	●	●	●
Energy Levels	●	●	●	●	●	●	●	●
Lifetimes	●	●	●		●		●	●
Ionization Limits	●	●	●	●	●	●		●
Photoionization Cross Sections	●	●	●	●	●	●		●
Multiphoton Cross Sections	●	●	●	●	●		●	●
Recombination Rates	●	●	●		●			●
Isotope Shifts	●	●	●	●	●	●	●	●
Hyperfine Splittings	●	●	●		●		●	●
External Field Effects	●	●	●		●	●	●	●
Collisional Properties	●	●	●		●			●

TABLE II : DATA NEEDS OF VARIOUS AREAS OF SOCIETY

70 *CURRENT TRENDS IN ATOMIC SPECTROSCOPY*

**LIST OF ABBREVIATIONS USED IN APPENDICES**

AD = Atomic Data  
ADNDT = Atomic Data and Nuclear Data Tables  
JILA = Joint Institute for Laboratory Astrophysics  
JPCRD = Journal of Physical and Chemical Reference Data  
NASA = National Aeronautics and Space Administration  
NBS = National Bureau of Standards  
NRL = Naval Research Laboratory  
NSRDS-NBS = National Standard Reference Data Series, National Bureau of Standards  
ORNL = Oak Ridge National Laboratory

APPENDIX A  
COMPILATIONS OF ATOMIC DATA

## I. WAVELENGTHS

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**15. WORK IN PROGRESS**

Atomic Energy Levels Data Center—NBS: energy levels of phosphorus, sulfur; revision of energy-level tables for the elements potassium through nickel

J. Blaise and co-workers (Laboratoire Aimé Cotton, Orsay, France): compilation of energy levels of the actinides

Data Center on Atomic Transition Probabilities—NBS: revision of transition-probability tables for allowed and forbidden transitions of the elements scandium through nickel

N. Konjevic (Institute of Physics, Beograd, Yugoslavia) and W. L. Wiese (NBS): updating of critical review of Stark widths and shifts for non-hydrogenic spectral lines of ionized atoms

C. E. Moore-Sitterly (NBS and NRL): multiplet table and energy levels for O III

National Space Science Data Center/World Data Center A for Rockets and Satellites—NASA: computerization of NSRDS-NBS 3, Sects. 1-9, "Selected Tables of Atomic Spectra" by C. E. Moore, to create a machine-readable finding list by ion

Spectroscopic Data Center—Naval Postgraduate School: updating of data tables of spectral lines of hydrogen through krypton in the ultraviolet, including energy levels

**APPENDIX B  
ATOMIC DATA CENTERS**

Name of Center: Atomic Collision Cross Sections Data Center  
Mailing Address: Joint Institute for Laboratory Astrophysics  
University of Colorado  
Campus Box 440  
Boulder, Colorado 80309  
Telephone: (303) 492-8089  
FTS: 320-3181  
Director: Jean W. Gallagher  
Scope: Compiles, evaluates, and disseminates data concerning electron and photon collisions with atoms, simple molecules, ions, and low-energy heavy particles. Emphasis is given to electron-collisional excitation and ionization, heavy-particle energy transfer, photoionization, photodetachment, and photofragmentation. Data on specific topics are evaluated by experts in the respective areas of interest. Responds to user requests for data, literature references, and technical information.

Name of Center: Atomic Energy Levels Data Center  
Mailing Address: National Bureau of Standards  
Building 221, Room A167  
Washington, DC 20234  
Telephone: (301) 921-2011  
FTS: 921-2011  
Director: William C. Martin, Jr.  
Contacts: Jack Sugar, Arlene F. Musgrove  
Scope: Collects, catalogs, and evaluates data on atomic energy levels, wavelengths, and ionization potentials of atoms and atomic ions in the gas phase. Publishes tables of critically evaluated data, as well as annotated bibliographies. Responds to user requests for data, literature references, and technical information.

Name of Center: Data Center on Atomic Transition Probabilities  
Mailing Address: National Bureau of Standards  
Building 221, Room A267  
Washington, DC 20234  
Telephone: (301) 921-2071  
FTS: 921-2071  
Director: Wolfgang L. Wiese  
Contacts: Georgia A. Martin, Jeffrey R. Fuhr  
Scope: Collects, catalogs, and evaluates data on transition probabilities and oscillator strengths of atoms and atomic ions in the gas phase, as well as radiative lifetimes of atomic and ionic levels. (Also, a collection of atomic line shapes and shifts resides here, but is no longer being kept current.) Publishes critical reviews and tables of critically evaluated data, as well as annotated bibliographies. Responds to

user requests for data, literature references, and technical information.

Name of Center: National Space Science Data Center/World Data Center A for  
Rockets and Satellites  
Mailing Address: Code 601  
National Aeronautics and Space Administration  
Goddard Space Flight Center  
Greenbelt, Maryland 20771  
Telephone: (301) 344-8310  
FTS: 344-8310  
Contact: Wayne H. Warren, Jr.  
Scope: Collects and distributes atomic spectroscopic data of interest to  
astronomers and astrophysicists. Some work is done on compiling  
finding lists of atomic lines. All data are in machine-readable form.  
Responds to user requests for data.

Name of Center: Spectroscopic Data Center  
Mailing Address: Code 61KE  
Naval Postgraduate School  
Monterey, California 93940  
Telephone: (408) 646-2824  
Autovon: 878-2824  
Director: Raymond L. Kelly  
Scope: Collects, evaluates, and publishes semicritical compilations of data  
on spectral lines of atoms and atomic ions in the gas phase. Col-  
lects and compiles energy-level data, which, along with classifica-  
tions of spectral lines, are included in published compilations. Cov-  
erage is limited to the elements hydrogen through krypton, and to  
the wavelength range below 3500 Å. Responds to user requests by  
circulating magnetic tapes of spectral data.

**APPENDIX C  
BIBLIOGRAPHIES ON ATOMIC SPECTROSCOPIC QUANTITIES**

**1. ATOMIC LINE SHAPES AND SHIFTS**

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**2. ENERGY LEVELS, WAVELENGTHS, IONIZATION POTENTIALS**

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#### 5. TRANSITION PROBABILITIES, OSCILLATOR STRENGTHS, LINE STRENGTHS, LIFETIMES

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#### 6. X-RAY TABULATIONS

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#### 7. MULTIPHOTON PROCESSES

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**APPENDIX D  
NEWSLETTERS**

- Name: Atomic Data for Fusion (bimonthly)  
Editors: D. H. Crandall and C. F. Barnett    W. L. Wiese  
Oak Ridge National Laboratory    National Bureau of Standards  
P. O. Box X, Bldg. 6003    Room A267, Building 221  
Oak Ridge, Tennessee 37830    Washington, DC 20234
- Scope: Atomic energy levels, wavelengths, transition probabilities, and atomic collision processes. References to published work; descriptions of work in progress; selected data.  
[Note: as of early 1982 this newsletter has been discontinued, and the input will be sent directly to the International Atomic Energy Agency for inclusion in their bulletin (see below).]
- Name: Information Quarterly for Atomic Processes and Applications  
Editors: W. Eissner and C. J. Noble  
Daresbury Laboratory  
Science and Engineering Research Council  
Daresbury, Warrington WA4-4AD  
England
- Scope: Continuum processes involving electron and photon collisions with atoms and molecules, including processes that occur in the presence of external electric and magnetic fields; photon- and electron-impact ionization; applications of atomic and molecular physics to solar physics problems. Primarily descriptions of work in progress.
- Name: International Bulletin on Atomic and Molecular Data for Fusion (quarterly)  
Editor: K. Katsonis  
Atomic and Molecular Data Unit  
Nuclear Data Section  
International Atomic Energy Agency  
Wagramerstrasse 5  
P. O. Box 100  
A-1400 Vienna, Austria
- Scope: Structure and spectra; collisions; surface effects. References to published work.